

## Useful information:

### VALUES OF SOME PHYSICAL CONSTANTS

| <i>Constant</i>                             | <i>Symbol</i>                    | <i>Value</i>   |
|---|----------------------------------|--|
| Avogadro's number                           | $N_0$                            | $6.02205 \times 10^{23} \text{ mol}^{-1}$  |
| Proton charge                               | $e$                              | $1.60219 \times 10^{-19} \text{ C}$  |
| Planck's constant                           | $h$<br>$\hbar$                   | $6.62618 \times 10^{-34} \text{ J}\cdot\text{s}$<br>$1.05459 \times 10^{-34} \text{ J}\cdot\text{s}$   |
| Speed of light in vacuum                    | $c$                              | $2.997925 \times 10^8 \text{ m}\cdot\text{s}^{-1}$   |
| Atomic mass unit                            | amu                              | $1.66056 \times 10^{-27} \text{ kg}$   |
| Electron rest mass                          | $m_e$                            | $9.10953 \times 10^{-31} \text{ kg}$   |
| Proton rest mass                            | $m_p$                            | $1.67265 \times 10^{-27} \text{ kg}$   |
| Boltzmann constant                          | $k_B$                            | $1.38066 \times 10^{-23} \text{ J}\cdot\text{K}^{-1}$<br>$0.69509 \text{ cm}^{-1}$   |
| Molar gas constant                          | $R$                              | $8.31441 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$  |
| Permittivity of a vacuum                    | $\epsilon_0$<br>$4\pi\epsilon_0$ | $8.854188 \times 10^{-12} \text{ C}^2\cdot\text{s}^2\cdot\text{kg}^{-1}\cdot\text{m}^{-3}$<br>$1.112650 \times 10^{-10} \text{ C}^2\cdot\text{s}^2\cdot\text{kg}^{-1}\cdot\text{m}^{-3}$ |
| Rydberg constant<br>(infinite nuclear mass) | $R_\infty$                       | $2.179914 \times 10^{-23} \text{ J}$<br>$1.097373 \text{ cm}^{-1}$   |
| First Bohr radius                           | $a_0$                            | $5.29177 \times 10^{-11} \text{ m}$  |
| Bohr magneton                               | $\mu_B$                          | $9.27409 \times 10^{-24} \text{ J}\cdot\text{T}^{-1}$  |
| Stefan-Boltzmann constant                   | $\sigma$                         | $5.67032 \times 10^{-8} \text{ J}\cdot\text{m}^{-2}\cdot\text{K}^{-4}\cdot\text{s}^{-1}$   |

The product rule says that

$$\frac{d}{dx}(fg) = f \frac{dg}{dx} + \frac{df}{dx}g,$$

from which it follows that

$$\int_a^b f \frac{dg}{dx} dx = - \int_a^b \frac{df}{dx} g dx + fg \Big|_a^b.$$

### Harmonic Oscillator:

$$\psi_n(x) = \sqrt{\frac{1}{2^n n!}} \cdot \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \cdot e^{-\frac{m\omega x^2}{2\hbar}} \cdot H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right)$$

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} (e^{-x^2})$$

### Some Potentially Useful Integrals:

$$\int_0^a x(a-x) \sin\left(\frac{n\pi}{a}x\right) dx = 2\left[\frac{a}{n\pi}\right]^3 [1 - \cos n\pi]$$

$$\int \sin^2(kx) dx = \frac{1}{2}x - \frac{1}{4k}\sin(2kx) + \text{constant}$$

$$\int_0^a x \sin^2\left(\frac{n\pi}{a}x\right) dx = \frac{a^2}{4}$$

$$\int_0^a x^2 \sin^2\left(\frac{n\pi}{a}x\right) dx = \left(\frac{a}{2\pi n}\right)^3 \left(\frac{4\pi^3 n^3}{3} - 2n\pi\right)$$

$$\int \cos^2 y dy = \frac{1}{2}y + \frac{1}{4}\sin 2y + \text{constant}$$

## SOME MATHEMATICAL FORMULAS

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$$\sin \alpha \sin \beta = \frac{1}{2} \cos (\alpha - \beta) - \frac{1}{2} \cos (\alpha + \beta)$$

$$\cos \alpha \cos \beta = \frac{1}{2} \cos (\alpha - \beta) + \frac{1}{2} \cos (\alpha + \beta)$$

$$\sin \alpha \cos \beta = \frac{1}{2} \sin (\alpha + \beta) + \frac{1}{2} \sin (\alpha - \beta)$$

$$\sin (\alpha \pm \beta) = \sin \alpha \cos \beta \pm \cos \alpha \sin \beta$$

$$\cos (\alpha \pm \beta) = \cos \alpha \cos \beta \mp \sin \alpha \sin \beta$$

$$e^{\pm i\theta} = \cos \theta \pm i \sin \theta$$

$$\cos \theta = \frac{e^{i\theta} + e^{-i\theta}}{2}$$

$$\sin \theta = \frac{e^{i\theta} - e^{-i\theta}}{2i}$$

$$f(x) = f(a) + f'(a)(x - a) + \frac{1}{2!} f''(a)(x - a)^2 + \frac{1}{3!} f'''(a)(x - a)^3 + \cdots$$

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + \cdots$$

$$\cos x = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \cdots$$

$$\sin x = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \cdots$$

$$\frac{1}{1 - x} = 1 + x + x^2 + x^3 + x^4 + \cdots \quad x^2 < 1$$

$$(1 \pm x)^n = 1 \pm nx + \frac{n(n-1)}{2!} x^2 \pm \frac{n(n-1)(n-2)}{3!} x^3 + \cdots \quad x^2 < 1$$

$$\int_0^\infty x^n e^{-ax} dx = \frac{n!}{a^{n+1}} \quad (n \text{ positive integer})$$

$$\int_0^\infty e^{-ax^2} dx = \left( \frac{\pi}{4a} \right)^{1/2}$$

$$\int_0^\infty x^{2n} e^{-ax^2} dx = \frac{1 \cdot 3 \cdot 5 \cdots (2n-1)}{2^{n+1} a^n} \left( \frac{\pi}{a} \right)^{1/2} \quad (n \text{ positive integer})$$

$$\int_0^\infty x^{2n+1} e^{-ax^2} dx = \frac{n!}{2a^{n+1}} \quad (n \text{ positive integer})$$

$$\int_0^a \sin \frac{n\pi x}{a} \sin \frac{m\pi x}{a} dx = \int_0^a \cos \frac{n\pi x}{a} \cos \frac{m\pi x}{a} dx = \frac{a}{2} \delta_{nm}$$

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|                      |                       |                         |                            |                      |                         |                        |                       |                         |                        |                        |                        |  |  |  |  |                         |                     |                       |                       |                      |                   |
|----------------------|-----------------------|-------------------------|----------------------------|----------------------|-------------------------|------------------------|-----------------------|-------------------------|------------------------|------------------------|------------------------|--|--|--|--|-------------------------|---------------------|-----------------------|-----------------------|----------------------|-------------------|
| hydrogen<br>1<br>H   | helium<br>2<br>He     |                         |                            |                      |                         |                        |                       |                         |                        |                        |                        |  |  |  |  |                         |                     |                       |                       |                      |                   |
| 1.0079               | 4.0026                |                         |                            |                      |                         |                        |                       |                         |                        |                        |                        |  |  |  |  |                         |                     |                       |                       |                      |                   |
| lithium<br>3<br>Li   | beryllium<br>4<br>Be  |                         |                            |                      |                         |                        |                       |                         |                        |                        |                        |  |  |  |  |                         |                     |                       |                       |                      |                   |
| 6.941                | 9.0122                |                         |                            |                      |                         |                        |                       |                         |                        |                        |                        |  |  |  |  |                         |                     |                       |                       |                      |                   |
| sodium<br>11<br>Na   | magnesium<br>12<br>Mg |                         |                            |                      |                         |                        |                       |                         |                        |                        |                        |  |  |  |  |                         |                     |                       |                       |                      |                   |
| 22.990               | 24.305                |                         |                            |                      |                         |                        |                       |                         |                        |                        |                        |  |  |  |  |                         |                     |                       |                       |                      |                   |
| potassium<br>19<br>K | calcium<br>20<br>Ca   |                         |                            |                      |                         |                        |                       |                         |                        |                        |                        |  |  |  |  |                         |                     |                       |                       |                      |                   |
| 39.098               | 40.078                |                         |                            |                      |                         |                        |                       |                         |                        |                        |                        |  |  |  |  |                         |                     |                       |                       |                      |                   |
| rubidium<br>37<br>Rb | strontium<br>38<br>Sr |                         |                            |                      |                         |                        |                       |                         |                        |                        |                        |  |  |  |  |                         |                     |                       |                       |                      |                   |
| 85.468               | 87.62                 |                         |                            |                      |                         |                        |                       |                         |                        |                        |                        |  |  |  |  |                         |                     |                       |                       |                      |                   |
| cesium<br>55<br>Cs   | barium<br>56<br>Ba    |                         |                            |                      |                         |                        |                       |                         |                        |                        |                        |  |  |  |  |                         |                     |                       |                       |                      |                   |
| 132.91               | 137.33                |                         |                            |                      |                         |                        |                       |                         |                        |                        |                        |  |  |  |  |                         |                     |                       |                       |                      |                   |
| francium<br>87<br>Fr | radium<br>88<br>Ra    |                         |                            |                      |                         |                        |                       |                         |                        |                        |                        |  |  |  |  |                         |                     |                       |                       |                      |                   |
| 1223                 | 1226                  |                         |                            |                      |                         |                        |                       |                         |                        |                        |                        |  |  |  |  |                         |                     |                       |                       |                      |                   |
|                      |                       | scandium<br>21<br>Sc    | titanium<br>22<br>Ti       | vanadium<br>23<br>V  | chromium<br>24<br>Cr    | manganese<br>25<br>Mn  | iron<br>26<br>Fe      | cobalt<br>27<br>Co      | nickel<br>28<br>Ni     | copper<br>29<br>Cu     | zinc<br>30<br>Zn       |  |  |  |  | boron<br>5<br>B         | carbon<br>6<br>C    | nitrogen<br>7<br>N    | oxygen<br>8<br>O      | fluorine<br>9<br>F   | neon<br>10<br>Ne  |
|                      |                       | 44.956                  | 47.867                     | 50.942               | 51.996                  | 54.938                 | 55.845                | 58.933                  | 58.693                 | 63.546                 | 65.39                  |  |  |  |  | 10.811                  | 12.011              | 14.007                | 15.999                | 18.998               | 20.180            |
|                      |                       | yttrium<br>39<br>Y      | zirconium<br>40<br>Zr      | niobium<br>41<br>Nb  | molybdenum<br>42<br>Mo  | technetium<br>43<br>Tc | ruthenium<br>44<br>Ru | rhodium<br>45<br>Rh     | palladium<br>46<br>Pd  | silver<br>47<br>Ag     | cadmium<br>48<br>Cd    |  |  |  |  | aluminum<br>13<br>Al    | silicon<br>14<br>Si | phosphorus<br>15<br>P | sulfur<br>16<br>S     | chlorine<br>17<br>Cl | argon<br>18<br>Ar |
|                      |                       | 88.906                  | 91.224                     | 92.906               | 95.94                   | [98]                   | 101.07                | 102.91                  | 106.42                 | 107.87                 | 112.41                 |  |  |  |  | 26.982                  | 28.086              | 30.974                | 32.065                | 35.453               | 39.948            |
|                      |                       | lutetium<br>71<br>Lu    | hafnium<br>72<br>Hf        | tantalum<br>73<br>Ta | tungsten<br>74<br>W     | rhenium<br>75<br>Re    | osmium<br>76<br>Os    | iridium<br>77<br>Ir     | platinum<br>78<br>Pt   | gold<br>79<br>Au       | mercury<br>80<br>Hg    |  |  |  |  | germanium<br>32<br>Ge   | tin<br>50<br>Sn     | antimony<br>51<br>Sb  | tellurium<br>52<br>Te | iodine<br>53<br>I    | xenon<br>54<br>Xe |
|                      |                       | 174.97                  | 178.49                     | 180.95               | 183.84                  | 186.21                 | 190.23                | 192.22                  | 196.08                 | 196.97                 | 200.59                 |  |  |  |  | 72.61                   | 118.71              | 121.76                | 127.60                | 126.90               | 131.29            |
|                      |                       | lawrencium<br>103<br>Lr | rutherfordium<br>104<br>Rf | dubnium<br>105<br>Db | seaborgium<br>106<br>Sg | bohrium<br>107<br>Bh   | hassium<br>108<br>Hs  | meitnerium<br>109<br>Mt | unnilium<br>110<br>Uun | unnilium<br>111<br>Uun | unnilium<br>112<br>Uub |  |  |  |  | lead<br>82<br>Pb        | bismuth<br>83<br>Bi | polonium<br>84<br>Po  | astatine<br>85<br>At  | radon<br>86<br>Rn    |                   |
|                      |                       | [262]                   | [261]                      | [262]                | [263]                   | [264]                  | [265]                 | [266]                   | [271]                  | [272]                  | [277]                  |  |  |  |  | 207.2                   | 208.98              | [209]                 | [210]                 | [222]                |                   |
|                      |                       |                         |                            |                      |                         |                        |                       |                         |                        |                        |                        |  |  |  |  | unquadium<br>114<br>Uuq |                     |                       |                       |                      |                   |
|                      |                       |                         |                            |                      |                         |                        |                       |                         |                        |                        |                        |  |  |  |  |                         |                     |                       |                       |                      |                   |

\*Lanthanide series

\*\*Actinide series

The solution is

$$\Theta(\theta) = AP_l^m(\cos \theta), \quad [4.26]$$

where  $P_l^m$  is the **associated Legendre function**, defined by

$$P_l^m(x) \equiv (1-x^2)^{|m|/2} \left( \frac{d}{dx} \right)^{|m|} P_l(x), \quad [4.27]$$

and  $P_l(x)$  is the  $l$ th **Legendre polynomial**, defined by the **Rodrigues formula**:

$$P_l(x) \equiv \frac{1}{2^l l!} \left( \frac{d}{dx} \right)^l (x^2 - 1)^l. \quad [4.28]$$

$$Y_l^m(\theta, \phi) = \epsilon \sqrt{\frac{(2l+1)}{4\pi} \frac{(l-|m|)!}{(l+|m|)!}} e^{im\phi} P_l^m(\cos \theta), \quad [4.32]$$

where  $\epsilon = (-1)^m$  for  $m \geq 0$  and  $\epsilon = 1$  for  $m \leq 0$ .

**TABLE 4.3:** The first few spherical harmonics,  $Y_l^m(\theta, \phi)$ .

|  |   |
|--|---|
| $Y_0^0 = \left(\frac{1}{4\pi}\right)^{1/2}$  | $Y_2^{\pm 2} = \left(\frac{15}{32\pi}\right)^{1/2} \sin^2 \theta e^{\pm 2i\phi}$                        |
| $Y_1^0 = \left(\frac{3}{4\pi}\right)^{1/2} \cos \theta$                                      | $Y_3^0 = \left(\frac{7}{16\pi}\right)^{1/2} (5 \cos^3 \theta - 3 \cos \theta)$                          |
| $Y_1^{\pm 1} = \mp \left(\frac{3}{8\pi}\right)^{1/2} \sin \theta e^{\pm i\phi}$              | $Y_3^{\pm 1} = \mp \left(\frac{21}{64\pi}\right)^{1/2} \sin \theta (5 \cos^2 \theta - 1) e^{\pm i\phi}$ |
| $Y_2^0 = \left(\frac{5}{16\pi}\right)^{1/2} (3 \cos^2 \theta - 1)$                           | $Y_3^{\pm 2} = \left(\frac{105}{32\pi}\right)^{1/2} \sin^2 \theta \cos \theta e^{\pm 2i\phi}$           |
| $Y_2^{\pm 1} = \mp \left(\frac{15}{8\pi}\right)^{1/2} \sin \theta \cos \theta e^{\pm i\phi}$ | $Y_3^{\pm 3} = \mp \left(\frac{35}{64\pi}\right)^{1/2} \sin^3 \theta e^{\pm 3i\phi}$                    |

**TABLE 4.7:** The first few radial wave functions for hydrogen,  $R_{nl}(r)$ .

|  |
|--|
| $R_{10} = 2a^{-3/2} \exp(-r/a)$  |
| $R_{20} = \frac{1}{\sqrt{2}} a^{-3/2} \left(1 - \frac{1}{2} \frac{r}{a}\right) \exp(-r/2a)$  |
| $R_{21} = \frac{1}{\sqrt{24}} a^{-3/2} \frac{r}{a} \exp(-r/2a)$  |
| $R_{30} = \frac{2}{\sqrt{27}} a^{-3/2} \left(1 - \frac{2}{3} \frac{r}{a} + \frac{2}{27} \left(\frac{r}{a}\right)^2\right) \exp(-r/3a)$                                   |
| $R_{31} = \frac{8}{27\sqrt{6}} a^{-3/2} \left(1 - \frac{1}{6} \frac{r}{a}\right) \left(\frac{r}{a}\right) \exp(-r/3a)$   |
| $R_{32} = \frac{4}{81\sqrt{30}} a^{-3/2} \left(\frac{r}{a}\right)^2 \exp(-r/3a)$   |
| $R_{40} = \frac{1}{4} a^{-3/2} \left(1 - \frac{3}{4} \frac{r}{a} + \frac{1}{8} \left(\frac{r}{a}\right)^2 - \frac{1}{192} \left(\frac{r}{a}\right)^3\right) \exp(-r/4a)$ |
| $R_{41} = \frac{\sqrt{5}}{16\sqrt{3}} a^{-3/2} \left(1 - \frac{1}{4} \frac{r}{a} + \frac{1}{80} \left(\frac{r}{a}\right)^2\right) \frac{r}{a} \exp(-r/4a)$               |
| $R_{42} = \frac{1}{64\sqrt{5}} a^{-3/2} \left(1 - \frac{1}{12} \frac{r}{a}\right) \left(\frac{r}{a}\right)^2 \exp(-r/4a)$  |
| $R_{43} = \frac{1}{768\sqrt{35}} a^{-3/2} \left(\frac{r}{a}\right)^3 \exp(-r/4a)$  |

**TABLE 4.5:** The first few Laguerre polynomials,  $L_q(x)$ .

|  |
|--|
| $L_0 = 1$  |
| $L_1 = -x + 1$   |
| $L_2 = x^2 - 4x + 2$   |
| $L_3 = -x^3 + 9x^2 - 18x + 6$                                  |
| $L_4 = x^4 - 16x^3 + 72x^2 - 96x + 24$                         |
| $L_5 = -x^5 + 25x^4 - 200x^3 + 600x^2 - 600x + 120$            |
| $L_6 = x^6 - 36x^5 + 450x^4 - 2400x^3 + 5400x^2 - 4320x + 720$ |

**TABLE 4.6:** Some associated Laguerre polynomials,  $L_{q-p}^p(x)$ .

|                           |                               |
|---------------------------|-------------------------------|
| $L_0^0 = 1$               | $L_0^2 = 2$                   |
| $L_1^0 = -x + 1$          | $L_1^2 = -6x + 18$            |
| $L_2^0 = x^2 - 4x + 2$    | $L_2^2 = 12x^2 - 96x + 144$   |
| $L_0^1 = 1$               | $L_0^3 = 6$                   |
| $L_1^1 = -2x + 4$         | $L_1^3 = -24x + 96$           |
| $L_2^1 = 3x^2 - 18x + 18$ | $L_2^3 = 60x^2 - 600x + 1200$ |