Useful constants and equations

Units and Constants:

Mass of an electron: $9.1094 * 10^{-31}$ kg = $5.4858 * 10^{-4}$ Da = 0.5110 MeV
Charge of an electron (e): $-1.6022 * 10^{-19}$ C
Mass of a free proton: $1.6726 * 10^{-27}$ kg = 1.0073 Da = 938.28 MeV
Mass of a free neutron: $1.6749 * 10^{-27}$ kg = 1.0087 Da = 939.57 MeV
1 atomic mass unit = 1/12 ^{12}C atomic mass = 1 Da ≈ $1.6605 * 10^{-27}$ kg = 931.494 MeV
1 Th = 1 Da/e = $1.0364*10^{-8}$ kg/C
1 J = 0.239006 calories = 1 N*m = 1 kg * m^2 / s^2
1 V = 1 J/C
1 coulomb (C) = $6.2415 * 10^{18}$ e (e is the charge on a single electron)
1 electron volt (eV) = $1.6022 * 10^{-19}$ J = 23.06 kcal/mole = 8065.54 cm^{-1} = 96.485 kJ/mol ≈ 11,600 K
1 MeV = $1.0 * 10^6$ eV = $1.6022 * 10^{-13}$ J
1 kcal/mol = 4.184 kJ/mole = 0.04336 eV = 349.75 cm^{-1}
Planck's constant (h) = $6.636 * 10^{-34}$ J * s
1 amp (A) = 1 C/second
Faraday constant (F) = $9.6485 * 10^4$ C/mole
1 hartree (E_h) = $4.3597 * 10^{-18}$ J = 27.211 eV
k = $1.3807 * 10^{-23}$ J/K = $8.6173 * 10^{-5}$ eV/K
at room temperature (293 K), kT = $4.045 * 10^{-21}$ J = 2.436 kJ/mol = 0.0252 eV
1 Tesla (T) = 10,000 gauss = 1 kg / (C * s)
R = 8.3144 J / (mol * K) = 62.364 (L * torr) / (mol * K)

Equations:

Newton's second law: F = m * a
Where F is force, m is mass, and a is acceleration
(for the Newton, 1 N = 1 kg * m / s^2)

Kinematics equation: $s = v_0 * t + ½ * a * t^2$
Where s is distance traveled, v_0 is the initial velocity of the object, a is a constant acceleration, and t is time. For non-constant accelerations, differential equations must be used.

Lorentz Force: F = q* [E + (v x B)] = q* [E + v * B * (sinθ)]
Where F is the force, q is the charge on the molecule in C (sign of charge is critical), E is the electric field strength in V/m, v is the velocity vector of the ion in m/s, and B is the magnetic field strength in T; θ is the angle between the particle's velocity and the magnetic field (for perpendicular motion, θ = 90°).

Mean free path for molecules of an ideal gas:

$$\lambda = \frac{R * T}{\sqrt{2} * \pi * d^2 * N_a * P}$$

Where λ is the mean free path, R is the gas constant, T is temperature, d is the diameter of the particle, N_a is Avogadro's number, and P is pressure (for nitrogen gas @ 10^{-6} torr and 293 K, d ≈ 0.3 nm, λ ≈ 7.59 m) An excellent tutorial can be found at http://hyperphysics.phy-astr.gsu.edu/hbase/kinetic/menfre.html.

DeBroglie wavelength: $\lambda = h / (m * v)$

Where λ is the wavelength, h is Planck's constant, m is mass, and v is velocity.

Resolving power: $R = m/\Delta m$ and **Resolution:** $r = \Delta m/m$

Where m is the mass/charge ratio of the ion in question and Δm is the difference in mass to be resolved.

Relative error in parts per million: $\sigma = 10^6*(M_o - M_t)$

Where σ is the error in ppm, M_o is the observed mass and M_t is the theoretical mass.

Helpful websites:

http://webbook.nist.gov is a great resource for general information about more than 7,000 compounds. Information available includes molar mass, heats of formation, heat capacities, ion energetics, mass spectra, etc.

http://chemfacilities.chem.indiana.edu/facilities/masspec/instructions.htm is part of the mass spectrometry facility's website and has links to several useful reference materials. Also see the MS Links page of the MSF website as well.