

# Units and Constants in MedeA

## Contents

- *Units and Constants in MedeA*
  - *Units*
  - *Constants*

## 1 Units

| Quantity                     | Symbol | Units                    | SI units         |
|------------------------------|--------|--------------------------|------------------|
| <b>Amount</b>                | mol    | Mole                     | 1.0 mol          |
| <b>Capacitance</b>           | F      | Farad                    | 1.0 F            |
| <b>Electric Charge</b>       | C      | Coulomb                  | 1.0 C            |
| <b>Electric Conductance</b>  | S      | Siemens                  | 1.0 S            |
| <b>Electric Current</b>      | A      | Ampere                   | 1.0 A            |
| <b>Electric Potential</b>    | V      | Volt                     | 1.0 V            |
| <b>Electric Resistance</b>   | ohm    | Ohm                      | 1.0 ohm          |
| <b>Energy</b>                | E rel  | Rest Energy of Electron  | 8.187111E-14 J   |
|                              | Ha     | Hartree                  | 4.359748E-18 J   |
|                              | J      | Joule                    | 1.0 J            |
|                              | Ry     | Rydberg                  | 2.179874E-18 J   |
|                              | btu    | British Thermal Unit     | 1.054350E+03 J   |
|                              | cal    | Calorie                  | 4.184000E+00 J   |
|                              | eV     | Electronvolt             | 1.602177E-19 J   |
|                              | erg    | Erg                      | 1.000000E-07 J   |
| <b>Energy Density</b>        | Pa     | Pascal                   | 1.0 Pa           |
|                              | bar    | Bar                      | 100000.0 Pa      |
| <b>Force</b>                 | N      | Newton                   | 1.0 N            |
|                              | dyn    | Dyne                     | 1.000000E-05 N   |
| <b>Frequency</b>             | Hz     | Hertz                    | 1.0 Hz           |
| <b>Inductance</b>            | H      | Henry                    | 1.0 H            |
| <b>Length</b>                | Ang    | Angstrom                 | 1E-10 m          |
|                              | bohr   | Bohr                     | 5.291773E-11 m   |
|                              | ft     | Foot                     | 3.048000E-01 m   |
|                              | in     | Inch                     | 2.540000E-02 m   |
|                              | l rel  | Length Unit Relativistic | 3.861593E-13 m   |
|                              | m      | Meter                    | 1.0 m            |
|                              | mi     | Mile                     | 1.609344E+03 m   |
|                              | rd     | Rod                      | 5.029200E+00 m   |
|                              | ua     | Astronomical Unit        | 149598000000.0 m |
|                              | yd     | Yard                     | 9.144000E-01 m   |
| <b>Magnetic Flux</b>         | Wb     | Weber                    | 1.0 Wb           |
| <b>Magnetic Flux Density</b> | T      | Tesla                    | 1.0 T            |
| <b>Mass</b>                  | g      | Gram                     | 0.001 kg         |

Continued on next page

Table 1 – continued from previous page

|                        |       |                          |                            |
|------------------------|-------|--------------------------|----------------------------|
|                        | kg    | Kilogram                 | 1.0 kg                     |
|                        | lb    | Pound                    | 4.535924E-01 kg            |
|                        | t     | Ton                      | 1000.0 kg                  |
|                        | u     | Unified Stomic Mass Unit | 1.6605402E-27 kg           |
| <b>Moment of Force</b> | E rel | Rest Energy              | 8.187111E-14 J of electron |
|                        | Ha    | Hartree                  | 4.359748E-18 J             |
|                        | J     | Joule                    | 1.0 J                      |
|                        | Ry    | Rydberg                  | 2.179874E-18 J             |
|                        | btu   | British thermal unit     | 1.054350E+03 J             |
|                        | cal   | Calorie                  | 4.184000E+00 J             |
|                        | eV    | Electronvolt             | 1.602177E-19 J             |
|                        | erg   | Erg                      | 1.000000E-07 J             |
| <b>Plane Angle</b>     | °     | Degree                   | 1.745329E-02 rad           |
|                        | '     | Angular Minute           | 2.908882E-04 rad           |
|                        | rad   | Radian                   | 1.0 rad                    |
|                        | deg   | Degree                   | 1.745329E-02 rad           |
| <b>Power</b>           | W     | Watt                     | 1.0 watt                   |
| <b>Pressure</b>        | Pa    | Pascal                   | 1.0 Pa                     |
|                        | bar   | Bar                      | 100000.0 Pa                |
| <b>Solid Angle</b>     | sr    | Steradian                | 1.0 sr                     |
| <b>Temperature</b>     | K     | Kelvin                   | 1.0 K                      |
|                        | C     | Deg Celsius              | 1.0 K                      |
|                        | F     | Deg Fahrenheit           | 5.555556E-01 K             |
| <b>Time</b>            | d     | Day                      | 86400.0 s                  |
|                        | h     | Hour                     | 3600.0 s                   |
|                        | min   | Minute                   | 60.0 s                     |
|                        | s     | Second                   | 1.0 s                      |
| <b>Volume</b>          | L     | Liter                    | 1.0 s                      |

## 2 Constants

| Constant | Description                      | SI units  |
|----------|----------------------------------|---|
| Eh       | Hartree Energy                   | 4.359748E-18 J  |
| G        | Gravitational Constant           | 6.672590E-11 m <sup>3</sup> /(kg*s <sup>2</sup> )                 |
| Na       | Avogadro Constant                | 6.022137E+23 1/mol  |
| R        | Molar Gas Constant               | 8.314510E+00 m <sup>2</sup> *kg/(mol*K*s <sup>2</sup> )           |
| Ralpha   | Rydberg Constant                 | 1.097373E+07 1/m  |
| Vm       | Molar Volume of Ideal Gas        | 2.241410E-02 m <sup>3</sup> /mol                                  |
| a0       | Bohr Radius                      | 5.291773E-11 m  |
| alpha    | Fine Structure Constant          | 7.297353E-03 1  |
| atm      | Standard Atmosphere              | 101325.0 Pa   |
| c        | Speed of Light in Vacuum         | 299792458.0 m/s   |
| e        | Elementary Charge                | 1.602177E-19 C  |
| eps0     | Permittivity of Vacuum           | 8.854188E-12 A <sup>2</sup> *s <sup>4</sup> /(m <sup>3</sup> *kg) |
| gamma    | Euler's Constant                 | 5.772157E-01 1  |
| gn       | Standard Acceleration of Gravity | 9.806650E+00 m/s <sup>2</sup>                                     |
| h        | Planck Constant                  | 6.6260755E-34 m <sup>2</sup> *kg/s                                |
| hbar     | Planck Constant / 2pi            | 1.054573E-34 m <sup>2</sup> *kg/s                                 |
| k        | Boltzmann Constant               | 1.380658E-23 m <sup>2</sup> *kg/(K*s <sup>2</sup> )               |
| lambdac  | Compton Wavelength               | 2.426311E-12 m  |
| me       | Electron Mass                    | 9.109390E-31 kg   |
| mp       | Proton Mass                      | 1.672623E-27 kg   |
| mu0      | Permeability of Vacuum           | 1.256637E-06 m*kg/(A <sup>2</sup> *s <sup>2</sup> )               |
| re       | Classical Electron Radius        | 2.817941E-15 m  |
| ub       | Bohr Magneton                    | 9.274015E-24 m <sup>2</sup> *A                                    |