The atomic unit of energy

The atomic unit of energy is the Hartree. One Hartree is equal to:

$$1\ Ha = \frac{e^2}{4\pi\varepsilon_0 a_0}$$

where e is the charge on the electron, ε_0 is the vacuum permittivity and a_0 is the Bohr radius. Note that when all is Said and done this is nothing more than the potential energy of two charges at a distance of a Bohr radius from each other. Calculate the value of the Hartree in Joules and then write it also in eV. What is the relationship with the Rydberg constant?

The atomic unit of energy

Substituting in the standard values we find:

$$1\ Ha = \frac{(1.602\ x\ 10^{-19}\ C)^2}{4\pi(8.85\ x\ 10^{-12}\ N^{-1}C^2/m^2)(5.29\ \mathrm{x}\ 10^{-11}\ m)}$$

The value of the Hartree in Joules is:

$$1\ Ha = 4.36\ x\ 10^{-18}\ J$$

To calculate the value in eV we simply divide the value of Joules by the charge on an electron.

$$1\ Ha\ (eV) = \frac{4.36\ x\ 10^{-18}\ J}{1.602\ x\ 10^{-19}\ C} = 27.2\ eV$$

1 Hartree is equal to 2 R (the Rydberg constant).