Review: properties of the Bohr Atom Chem BC3253x

Classically: in two dimensions, using polar coordinates (r, θ)

object of mass m subject to a central potential $V(r) = -ZA/r$

for Coulomb's Law attraction, $A = e^2/4\pi\varepsilon_0$,

Z is the charge on the nucleus (in units of e)

The angular momentum, $\ell = mr^2(d\theta/dt)$ is constant.

If we assume circular orbits then

$E = -mA^2Z^2/2\ell^2$ and $r = \ell^2/mAz$

The old quantum theory: Bohr's theory says $\ell = n\hbar$

so $E_n = -mA^2Z^2/2n^2\hbar^2$ and $r_n = n^2\hbar^2/mAz$

If we define two constants:

$\mathbf{E_h} \equiv m_eA^2/\hbar^2$	and $\mathbf{a_0} \equiv \hbar^2/m_eA$
units: energy	units: length
called a **Hartree**	called a **Bohr**

(note that $E_h = \hbar^2/m_ea_0^2$)

Then (when $m = m_e$):

$E_n = -Z^2 E_h / 2n^2$ and $r_n = n^2 a_0 / Z$

When z=1 (H atom) and n=1(ground state)

$E_1 = -E_h/2$ and $r_1 = a_0$

The energy of ground state H atom is –½ Hartree. The magnitude of the hartree is twice the binding energy of the electron in a ground state H atom (equivalently, twice the ionization energy of ground state H).

The bohr is the radius of the orbit in a ground state H atom.

Hartrees and bohrs are **atomic units** of energy and length, respectively. They are used extensively by quantum chemists.

Using atomic units, the ground state of H has energy –½ and radius 1. The nth state of H atom has energy $-1/2n^2$ and radius n^2.

Relation to Rydberg constant R_∞: since $E_n = -hcR_\infty/n^2$, $E_h = 2\ hcR_\infty$