

### 3.5: Some Useful Expressions

Listed below are a number of equations which give the dependence of  $\bar{r}$ ,  $\overline{PE}$  and  $\overline{KE}$  on the quantum numbers  $n$ ,  $l$  and  $m$ . They refer not only to the hydrogen atom but also to any one-electron ion in general with a nuclear charge of  $Z$ . Thus  $\text{He}^+$  is a one-electron ion with  $Z = 2$ ,  $\text{Li}^{+2}$  another example with  $Z = 3$ .

The average distance between the electron and the nucleus expressed in atomic units of length is:

$$r_{n,l,m} = \frac{n^2}{Z} \left[ 1 + \frac{1}{2} \left\{ 1 - \frac{l(l+1)}{n^2} \right\} \right]$$

Note that  $\bar{r}_{n,l,m}$  is proportional to  $n^2$  for  $l = 0$  orbitals, and deviates only slightly from this for  $l \neq 0$ . The value of  $\bar{r}_{n,l,m}$  decreases as  $Z$  increases because the nuclear attractive force is greater. Thus  $\bar{r}_{1,0,0}$  for  $\text{He}^+$  would be only one half as large as  $\bar{r}_{1,0,0}$  for H.

$$E_n = -\frac{Z^2}{n^2} K = -\frac{Z^2}{2n^2} \text{ au}$$

$$K = \frac{2\pi^2 m e^4}{h^2} = \frac{e^2}{2a_0}$$

$$(\overline{PE})_{n,l,m} = -\frac{2Z^2}{n^2} K$$

$$(\overline{KE})_{n,l,m} = -E_n = +\frac{Z^2}{n^2} K$$

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