

6. Calculate $\langle r \rangle_{3d}$ for O^{7+} ion

$$\langle r \rangle = \langle R(r) \Theta(\theta) \Phi(\phi) | \hat{r} | R(r) \Theta(\theta) \Phi(\phi) \rangle$$

$$= \int_0^{\infty} r^3 R(r)^2 dr$$

Also *Show how!*
Check that this is dimensionally correct.

$$R_{3d}(r) = \frac{4}{81\sqrt{30}} Z^{7/2} r^2 e^{-Zr/3} \quad \text{in a.u. units}$$

$$\langle r \rangle = \frac{16}{81^2 \times 30} Z^7 \int_0^{\infty} r^7 e^{-2Zr/3} dr$$

$$= \frac{16}{81^2 \times 30} Z^7 \times \frac{7!}{\left(\frac{2Z}{3}\right)^8} = \frac{16 \times 7! \times 3^8}{81^2 \times 30 \times 2^8 \times Z}$$

$$= \frac{21}{2Z} \text{ a.u.}$$

$$= \frac{21}{16} \text{ a.u.} = 1.312 \text{ a.u.} = 1.312 \times 0.5292 \text{ \AA} = 0.694 \text{ \AA}$$

Calculate r_{max} for this orbital.