EM102. Nuage électronique de l'atome d'hydrogène

1. $$-e = \iiint \rho(r)\,d\tau = \int_{r=0}^{\infty}\int_{\theta=0}^{\pi}\int_{\varphi=0}^{2\pi} A e^{-2r/a_0}\, r^2 \sin\theta\, d\theta\, d\varphi\, dr$$

$$= 4\pi A \int_0^{\infty} r^2 e^{-2r/a_0}\, dr \,.$$ Posons $u = \frac{2r}{a_0}$; $dr = \frac{a_0}{2} du$.

$$\Rightarrow -e = 4\pi A \int_0^{\infty} \frac{a_0^3}{8} u^2 e^{-u}\, du$$

Calculons $$\int_0^{\infty} u^2 e^{-u} du \underset{IPP}{=} \left[-u^2 e^{-u}\right]_0^{\infty} + \int_0^{\infty} 2u e^{-u} du$$

$$\underset{IPP}{=} 0 + \left[-2u e^{-u}\right]_0^{\infty} + \int_0^{\infty} 2 e^{-u} du$$

$$= 0 + 0 + \left[-2e^{-u}\right]_0^{\infty} = +2$$

$$\Rightarrow -e = -\pi A a_0^3 \Rightarrow \boxed{A = -\frac{e}{\pi a_0^3}}$$

2. On cherche R tel que $$-\frac{95}{100} e = 4\pi A \frac{a_0^3}{8} \int_0^{U} u^2 e^{-u} du$$

où $U = \frac{2R}{a_0}$

$$\Rightarrow 1{,}9 = \int_0^{U} u^2 e^{-u} du \,.$$

$$= \left[-u^2 e^{-u}\right]_0^{U} - \left[2u e^{-u}\right]_0^{U} - \left[2e^{-u}\right]_0^{U}$$

$$= -U^2 e^{-U} - 2U e^{-U} - 2e^{-U} + 2$$

$$1{,}9 = 2 - (U^2 + 2U + 2)e^{-U}$$

$$(U^2 + 2U + 2)e^{-U} - 0{,}1 = 0 \xrightarrow[\text{résolution numérique}]{} U = 6{,}3 \rightarrow \underline{R = 3{,}1\, a_0}$$

$$\underline{R = 1{,}6\ \text{Å}}$$