Module chimie théorique — 2ème année

Question de cours

1 → c (1)
2 → b (1)
3 → a (1)
4 → a , b (1)
5 → a (1)
6 → a (1)

Exercice 1

1- $f(x) = \sin(x)$

$g(x) = \cos(x)$

$\hat{A} f(x) = g(x)$ (1)

$\Rightarrow \hat{A} \sin(x) = \cos(x)$

$\Rightarrow \frac{\partial}{\partial x} \sin(x) = \cos(x)$ (0,5)

$\hat{A} = \frac{\partial}{\partial x}$ (0,5)

2- $f(x) = \frac{\partial}{\partial x}$

$g(x) = x$

$\hat{A} f(x) = g(x)$

$\Rightarrow \hat{A} \frac{\partial}{\partial x} = x$ (0,5)

$\Rightarrow \int \frac{\partial}{\partial x} = x$

$\Rightarrow \hat{A} = \int$ (0,5)

3- $[\hat{A}, \hat{B}] \psi(x) = \hat{A}\hat{B}\psi(x) - \hat{B}\hat{A}\psi(x) = 0$ (1)

$\hat{A}\hat{B}\psi(x) = P_x \, x \, \psi(x)$ (0,5)

on a $P_x = -i\hbar \frac{\partial}{\partial x}$ (0,5)

$\hat{A}, \hat{B} \psi(x) = -i\hbar \frac{\partial}{\partial x} x \psi(x) = -i\hbar [\psi(x) + x\psi'(x)$ (0,5)

$\hat{B}, \hat{A} \psi(x) = x(-i\hbar \frac{\partial}{\partial x} \psi(x)) = -i\hbar (x \psi'(x))$ (0,5)

$[\hat{A}, \hat{B}] \psi(x) = -i\hbar \psi(x) \neq 0$ (0,5)

$[\hat{A}, \hat{B}]$ ne commutent pas (0,5)

Exo 2

l'orbitale 1s est $\varphi_{1s} = N_{1s} e^{-\frac{r}{a_0}}$

la constante N obtenu par la normalisation

$$\int \Psi \Psi^* dv = 1$$ (0,5)

$\langle \Psi | \Psi \rangle = 1$ selon Dirac (0,5)

1s est une sphère $V = \frac{4}{3}\pi r^3 \Rightarrow dv = 4\pi r^2$ (1) (1)

$$1 = 4\pi N_{1s}^2 \int r^2 e^{-2\frac{r}{a_0}} dr$$ (1)

On tient compte l'intégrale

$$\int x^n e^{-ax} dx = \frac{n!}{a^{n+1}} \quad (a>0)$$ (1)

$$1 = 4\pi N_{1s}^2 a^3 \Rightarrow N_{1s} = \frac{1}{\sqrt{\pi a_0^3}}$$ (1)

$$\Rightarrow \Psi_{1s} = \frac{1}{\sqrt{\pi a_0^3}} e^{-\frac{r}{a_0}}$$