CHEM 20100 (Inorganic Chemistry I) Notes

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Topics

Topic 0

Course Prep

0.1 Chapter 2: Atomic Structure

From Miessler et al., 2014.

0.1.1 Problems

2.8 The details of several steps in the particle-in-a-box model in this chapter have been omitted. Work out the details of the following steps:

a. Show that if $\Psi = A\sin rx + B\cos sx$ (A, B, r, and s are constants) is a solution to the wave equation for the one-dimensional box, then

$$r = s = \sqrt{2mE}\left(\frac{2\pi}{h}\right)$$

Solution.

$$\begin{aligned}
\frac{-h^2}{8\pi^2 m}\cdot\frac{\partial^2\Psi(x)}{\partial x^2}(A\sin rx + B\cos sx) &= E\Psi(x)\\
\frac{-h^2}{8\pi^2 m}\cdot\frac{\partial^2}{\partial x^2}(A\sin rx + B\cos sx) &= E(A\sin rx + B\cos sx)\\
\frac{-h^2}{8\pi^2 m}\cdot\frac{\partial}{\partial x}(Ar\cos rx - Bs\sin sx) &= E(A\sin rx + B\cos sx)\\
\frac{-h^2}{8\pi^2 m}\cdot\left(-Ar^2\sin rx - Bs^2\cos sx\right) &= E(A\sin rx + B\cos sx)\\
\frac{Ar^2h^2}{8\pi^2 m}\sin rx + \frac{Bs^2h^2}{8\pi^2 m}\cos sx &= AE\sin rx + BE\cos sx\\
0 &= \left(\frac{Ar^2h^2}{8\pi^2 m} - AE\right)\sin rx + \left(\frac{Bs^2h^2}{8\pi^2 m} - BE\right)\cos sx
\end{aligned}$$

Choose $x = 0$.

$$\begin{aligned}
&= \frac{Bs^2h^2}{8\pi^2 m} - BE\\
E &= \frac{s^2h^2}{8\pi^2 m}\\
\frac{8\pi^2 mE}{h^2} &= s^2\\
s &= \sqrt{\frac{8\pi^2 mE}{h^2}}
\end{aligned}$$

$$\boxed{s = \sqrt{2mE}\frac{2\pi}{h}}$$

With this result ...

$$\begin{aligned}
0 &= \left(\frac{Ar^2h^2}{8\pi^2 m} - AE\right)\sin rx + \left(\frac{Bs^2h^2}{8\pi^2 m} - BE\right)\cos sx \\
&= \left(\frac{Ar^2h^2}{8\pi^2 m} - AE\right)\sin rx + \left(B\left(\frac{s^2h^2}{8\pi^2 m}\right) - BE\right)\cos sx \\
&= \left(\frac{Ar^2h^2}{8\pi^2 m} - AE\right)\sin rx + (BE - BE)\cos sx \\
&= \left(\frac{Ar^2h^2}{8\pi^2 m} - AE\right)\sin rx
\end{aligned}$$

Choose $x = \frac{\pi}{2r}$.

$$\begin{aligned}
&= \frac{Ar^2h^2}{8\pi^2 m} - AE \\
&\boxed{r = \sqrt{2mE}\frac{2\pi}{h}}
\end{aligned}$$

□

d. Show that substituting the value of r given in part c into $\Psi = A\sin rx$ and applying the normalizing requirement gives $A = \sqrt{2/a}$.

Solution.

$$\begin{aligned}
1 &= \int_{\text{all space}} \Psi\Psi^* \,\mathrm{d}\tau \\
&= \int_0^a \left(A\sin\frac{n\pi x}{a}\right)\left(A\sin\frac{n\pi x}{a}\right)\mathrm{d}x \\
&= \int_0^a A^2\sin^2\frac{n\pi x}{a}\,\mathrm{d}x
\end{aligned}$$

Use $\sin^2 u = \frac{1-\cos 2u}{2}$.

$$\begin{aligned}
&= A^2\int_0^a \frac{1-\cos\frac{2n\pi x}{a}}{2}\,\mathrm{d}x \\
&= \frac{A^2}{2}\left(\int_0^a \mathrm{d}x - \int_0^a \cos\frac{2n\pi x}{a}\,\mathrm{d}x\right) \\
&= \frac{A^2}{2}\left([x]_0^a - \left[\frac{a}{2n\pi}\sin\frac{2n\pi x}{a}\right]_0^a\right) \\
&= \frac{A^2}{2}\left((a-0) - \left(\frac{a}{2n\pi}\sin 2n\pi - \frac{a}{2n\pi}\sin 0\right)\right) \\
&= \frac{A^2}{2}\left(a - \left(\frac{a}{2n\pi}\sin 2n\pi\right)\right)
\end{aligned}$$

Since n is an integer, $\sin 2n\pi = 0$.

$$\begin{aligned}
&= \frac{aA^2}{2} \\
\frac{2}{a} &= A^2 \\
&\boxed{A = \sqrt{\frac{2}{a}}}
\end{aligned}$$

□

References

Miessler, G. L., Fischer, P. J., & Tarr, D. A. (2014). *Inorganic chemistry* (fifth). Pearson Education.