CH1101 : Elements of Chemistry

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1. We have

$$P_{1s}(r) = 4\pi r^2 (\psi(r))^2$$
$$\psi_{1s}(r) = K \exp(-r/a_0)$$

Thus, for an electron in the 1s orbital, $P(r)$ increases, reaches a maxima, then decreases asymptotically to zero.

Although $\psi(r)$ is maximum at the nucleus, note that $r^2 \to 0$. Thus, for very small r,

$$P(r) \propto \lim_{r \to 0^+} r^2 \cdot \exp(-r) = 0$$

Conversely, for very large r, we take the limit

$$P(r) \propto \lim_{r \to \infty} r^2 \cdot \exp(-r) = 0$$

Here, we have used L'Hôpital's Rule.

The extrema of $P(r)$ occur at r such that

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}r} P(r) &= 0 \\ \frac{\mathrm{d}}{\mathrm{d}r} r^2 \cdot \exp(-2r/a_0) &= 0 \\ r &= a_0 \end{aligned}$$

Note that $\frac{\mathrm{d}^2}{\mathrm{d}r^2} P(r)$ at a_0 is negative, which means that $P(r)$ shows a maximum there.

2.

3. (i) The highest probability of finding an electron in the 3d orbital is closest to the nucleus, with $r/a_0 \approx 9$.
   (ii) At $r \approx 0.1a_0$, the probability of finding an electron is maximum for the 3s orbital.

4.

5. Let $x = r/a_0$. We have

$$R_{31} = N_{31}(6x - x^2)\exp(-x/3).$$

Cleary, the exponential part of this function never reaches zero. The quadratic part has its zeroes at 0 and 6. We thus know that the corresponding radial distribution function for the 3p orbital has a radial node at $r = 3a_0$.

(We ignore $r = 0$ *since the probability of finding an electron at the nucleus is meaningless.)*

6.

	Radial nodes	Angular nodes	Total nodes
1s	0	0	0
2s	1	0	1
2p	0	1	1
3s	2	0	2
3p	1	1	2

7. (i) This is a $3p_z$ orbital, with one radial node and one angular node.

(ii) a represents an angular node. b represents a radial node.

(iii) Each line in the contour plot is draw such that the probability of finding an electron on any point on that line is exactly the same. Thus, each line is an iso-probable curve. Red lines are drawn where the wavefunction of the electron is postive, and blue lines are drawn where the wavefunction is negative.

(iv) $c < d < e$, in order of the probability of finding an electron on that curve.

(v) $d > f$, by horizontal symmetry of the wavefunction.

8.