

Atomic Structure (Formula)

1. $E = -13.6 \frac{Z^2}{n^2} \text{ eV}$

2. $v = 2.18 \times 10^6 \frac{Z}{n} \text{ m/sec}$

3. $r = 0.529 \frac{n^2}{Z} \text{ \AA}$

4. $E(n) = -\frac{R_H}{n^2}$ $R_H = 2.18 \times 10^{-18}$

5. $\bar{\nu} = \frac{1}{\lambda} = R_H Z^2 \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right]$ (for $E_{\text{photon}} = h\nu = hc$)

7. $\lambda = \frac{h}{mv} = \frac{h}{\sqrt{2mKE}} = \frac{h}{\sqrt{2m_e V}}$ $\Delta V_{SP} = \sqrt{V_e - V_{SP}} = KE$

9. Photoelectric effect
 $h\nu = W_0 + \frac{1}{2}mv_e^2$

10. Heisenberg

i) $\Delta x \cdot \Delta p \geq \frac{h}{4\pi}$

11. $mvr = \frac{nh}{2\pi}$
↑
orbit ang. mom

ii) $\Delta x \cdot \Delta v \geq \frac{h}{4\pi m}$

iii) $\Delta E \cdot \Delta t \geq \frac{h}{4\pi}$

12. orbital ang. mom = $\sqrt{l(l+1)} \frac{h}{2\pi}$

13. total spin (S) = $\frac{1}{2} \times n \rightarrow$ no. of unpaired e⁻

14. spin magnetic moment = $\sqrt{n(n+2)} \text{ B.M.}$

15. Spin multiplicity = $2S+1$

16. total nodes = $n-1$

17. radial nodes = $n-l-1$

18. ang. nodes (N.P) = l

19. max type of wavelength = $\frac{n(n-1)}{2}$

20. total / max electron = $2n^2$
↳ orbit no.

Calculation Of Atomic Structures

Edward Neville da Costa Andrade



Calculation Of Atomic Structures:

The Calculation of Atomic Structures Douglas Rayner Hartree,1957 **The Calculation of Atomic Structures, Etc** Douglas Rayner Hartree,1957 Atomic Structure Theory Walter R. Johnson,2007-03-08 Atomic Structure Theory is a textbook for students with a background in quantum mechanics The text is designed to give hands on experience with atomic structure calculations Material covered includes angular momentum methods the central field Schrödinger and Dirac equations Hartree Fock and Dirac Hartree Fock equations multiplet structure hyperfine structure the isotope shift dipole and multipole transitions basic many body perturbation theory configuration interaction and correlation corrections to matrix elements Numerical methods for solving the Schrödinger and Dirac eigenvalue problems and the Dirac Hartree Fock equations are given as well B spline basis sets are used to carry out sums arising in higher order many body calculations Illustrative problems are provided together with solutions FORTRAN programs implementing the numerical methods in the text are included

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