*Basic Quantum Chemistry Reference*

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**Particle in a Box**

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3-Dimensional Particle in a Box

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**Harmonic Oscillator**

**Hermite Polynomials**

**Ladder Operators**

**;**

**;**

**The First Few Normalized Wave Functions**

**Alternate General Form of the Wave Function**

**Note that only even or only odd terms are included in the sum**

**For n = even,**

**For n = odd,**

**The entire wave function must be normalized after the summation**

**Rigid Rotor and Spherical Harmonics**

**Spherical Harmonics**

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**Angular Momentum Operators**

**Ladder Operators**

**Hydrogenic Atom**

**Wave Functions**

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| ****Complex Hydrogenic Wave Functions**** | |
| ***1s*** |  |
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| 3s |  |
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| ****Real Hydrogenic Wave Functions**** | |
| ***1s*** |  |
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| 3s |  |
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**Hamiltonian**

**Energies**

**Many Electron Atom**

**Wave Functions**

**Hamiltonian**

**Energies**

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| ****Term Symbols for Equivalent Electrons**** | |
| ***Configuration*** | **Terms** |
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| ****Term Symbols for Nonequivalent Electrons**** | |
| ***Configuration*** | **Terms** |
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**Variational Theory**

**Linear Variational Theory**

**Energies**

**To find En solve for W in the secular equation:**

**This gives roots of W, corresponding to the upper bounds of the m lowest energy states.**

**Wave Functions**

**To find and solve this system of equations:**

**Because the above system is not completely linearly independent (by one degree) we must finally normalize by:**

**Non-Degenerate Perturbation Theory**

**The First Few Degrees of Energy Correction**

**Degenerate Perturbation Theory**

**Finding Correct Zero-Order Wave Functions**

**To find , solve the secular equation:**

**The First Few Degrees of Energy Correction**

**Definite and Indefinite Integrals**

**Remember that**

**Physical Constants and** [Conversion](#_Hlk280014212)**s**

|  |  |  |  |
| --- | --- | --- | --- |
| ****Constant**** | ****Symbol**** | ****SI Value**** | ****Gaussian Value**** |
| **Speed of Light in Vacuum** | **c** |  |  |
| **Proton Charge** | **e** |  |  |
| **″** | **e'** |  |  |
| **Vacuum Permittivity** |  |  |  |
| **Avogadro Constant** |  |  |  |
| **Electron Rest Mass** |  |  |  |
| **Proton Rest Mass** |  |  |  |
| **Neutron Rest Mass** |  |  |  |
| **Planck Constant** | **ℎ** |  |  |
| **Reduced Planck Constant** | **ℏ** |  |  |
| **Faraday Constant** | **F** |  |  |
| **Vacuum Permeability** |  |  |  |
| **Bohr Radius** |  |  |  |
| **Bohr Magneton** |  |  |  |
| **Nuclear Magneton** |  |  |  |
| **Electron g Value** | **ge** |  |  |
| **Proton g Value** | **gp** |  |  |
| **Gas Constant** | **R** |  |  |
| **Boltzmann Constant** | **k** |  |  |
| **Gravitational Constant** | **G** |  |  |

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| ****Energy**** ****Conversion Factors**** |
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**Notes and Acknowledgements:**

1. Spherical coordinates are represented in the way standard for chemists (which is different from the standard used by mathematicians). i.e. r = radius from origin,  **angle with the positive z axis, angle between the positive x axis and the projection onto the x/y plane.**
2. While I have worked hard to ensure that this document is correct, I assume no responsibility for the accuracy of the information here.

The following were used in compiling this reference:

1. http://panda.unm.edu/Courses/Finley/P262/Hydrogen/WaveFcns.html
2. Levine, Ira N. *Quantum Chemistry 6th ed.* Pearson Prentice Hall (Upper Saddle River, NJ) 2009.
3. Hollas, J. Michael. *Modern Spectroscopy.* John Wiley & Sons, Ltd. (Chichester, West Sussex, England) 2004.