*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**

**Intro to Many Electron Atom**

**Wave Functions**

**For Ground State Solve the Slater Determinant:**

**Hamiltonian**

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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. **This reference sheet was written shortly after I finished an introductory quantum chemistry course in my senior year. It was originally meant to help me remember that course in years to come, and while the quality standards have increased the scope has remained the same. It will not likely be helpful at all to one who does not already understand how to use these equations.**
3. 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.