

# Quantum Number Calculator Using Python

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## Abstract

The "Quantum Number Calculator Using Python" is a computational tool designed to simplify determining quantum numbers— specifically principal ( $n$ ), angular momentum ( $l$ ), and magnetic ( $m$ )— in atomic structures. These quantum numbers are fundamental for understanding electron configurations and orbital distributions in chemistry.

This project automates the calculation of possible quantum numbers for a given principal quantum number, reducing manual effort and minimizing human errors. The program processes user input through logical conditions and displays valid quantum states alongside orbital shapes, enhancing the educational experience in fields like atomic physics, spectroscopy, and material science.

## Introduction

Quantum numbers are crucial for explaining the behaviour of electrons within atoms. Understanding these numbers helps students and researchers grasp core chemistry concepts like atomic orbitals, electron configuration, and chemical bonding.

This project integrates Python programming to create a quantum number calculator that provides an interactive, educational experience for learners.

## Objective

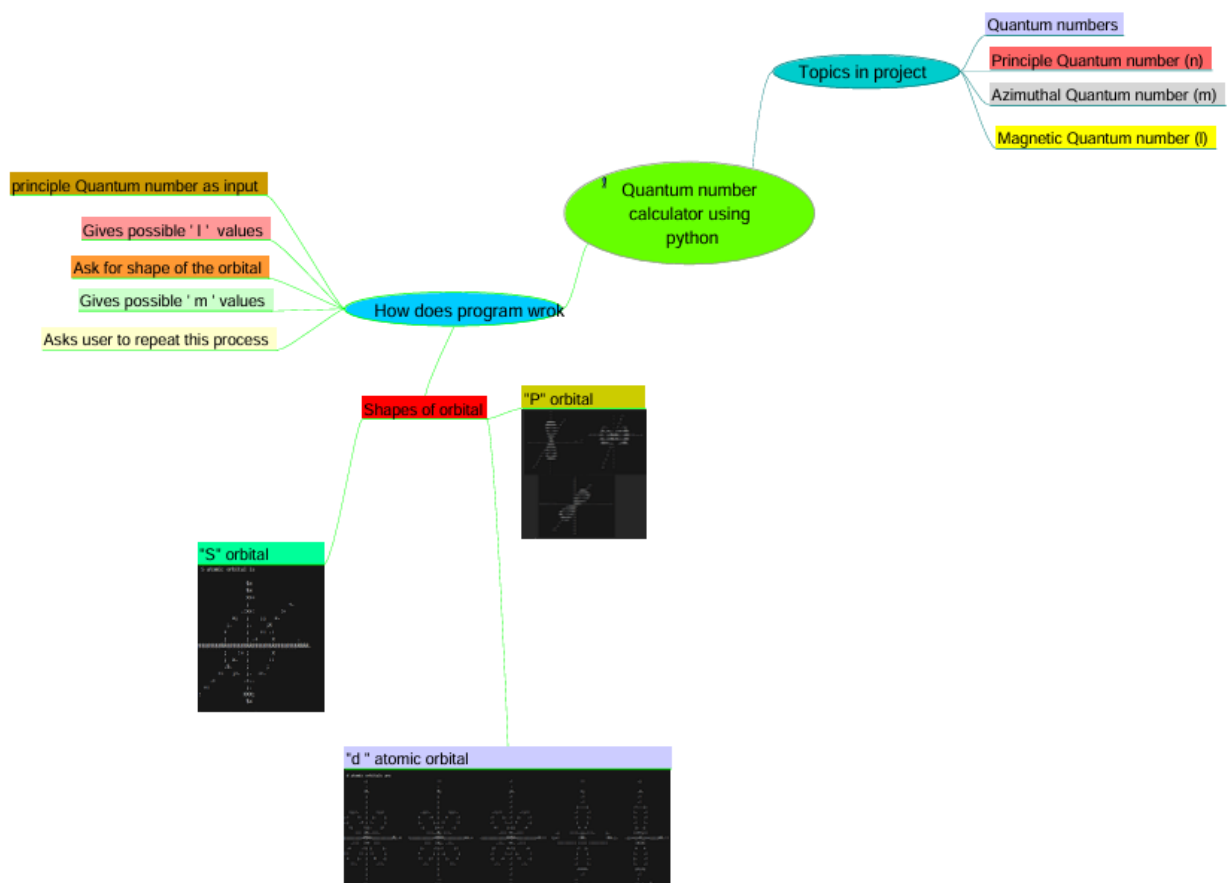
- Automate the calculation of valid quantum numbers for a given principal quantum number ( $n$ ).
- Display all possible ( $l$ ) and ( $m$ ) values along with corresponding orbital shapes.
- Enhance learning through computational chemistry tools.

## Methodology

The calculator is developed using Python, employing various programming concepts:

- **User Input Handling:** Using `input()` function to take user input.

- **Conditional Statements:** Using if-else blocks to validate input ranges for quantum numbers.
- **Loops:** for and while loops to generate all possible values.
- **Lists and Iteration:** To store and display the values of  $l$  and  $m$ .
- **String Formatting:** Using f-strings for structured and readable output.
- **Functions:** Modular coding via function `quantum()` for reusability.
- **External Modules:** Used modules like `art` and visualizations (e.g., Freeplane software) for depicting orbital structures.





# Installation & Setup Instructions

To run the Quantum Number Calculator on any system, follow these steps:

1. **Download and Install Python (v3.12.0 or later)**

Visit the official website: <https://www.python.org/downloads/>

2. **Running the Program**

- Extract the downloaded ZIP file containing the Python project.

## 1. Organize Your Files

Make sure the following files are in **the same folder**:

- Quantm.py
- art.py
- orbitals.py

For example, put them all in a folder named quantum\_project.

## ◇ 2. Open Your Terminal

- On **Windows**: Press Windows + R, type cmd, and press Enter.
- On **macOS**: Open Spotlight (Cmd + Space), type "Terminal", and press Enter.
- On **Linux**: Use Ctrl + Alt + T to open a terminal.

## ◇ 3. Navigate to Your Folder

Use the cd command to go into the folder where your .py files are located. For example:

```
cd Desktop/quantum_project
```

Replace the path with the actual location where you saved the files.

## ◇ 4. Run the Python Script

Now run the script using Python. Use one of the following commands:

```
python Quantm.py
```

or if your system uses python3:

```
python3 Quantm.py
```

Now, that code will start executing

## Features

- Simple and interactive user interface.
- Accurate generation of all valid quantum numbers.
- Integration of orbital shape representations.
- Modular code for easy maintenance and upgrades.

## Applications

- **Educational Purpose:** Helps students understand quantum mechanics visually and practically.
  - **Research Assistance:** Useful for researchers in atomic physics, spectroscopy, and material science.
  - **Learning Programming Concepts:** Demonstrates practical application of Python basics like loops, conditionals, and modularity.
- Conclusion

## Conclusion

The Quantum Number Calculator bridges the gap between theoretical chemistry concepts and practical computational tools. By automating tedious calculations, it provides an engaging way for learners to explore quantum numbers and their significance in atomic structure. This project demonstrates the powerful synergy between chemistry and programming, making complex concepts more accessible and understandable.