Chemistry Toolkit Technical Specification

Christopher Chang

Created On: 2024-03-18

Last Updated On: 2024-03-18

# Introduction

## Overview

Coding project for learning python. The goal is to provide a tool which can be used for computations that are commonly used in chemistry.

## Glossary

Valance

## Context

Request from Emma Storimans.

## Technical Requirements

Generated by ChatGPT on 2024-03-18.

1. Element Information Display:

* Display basic information about an element (atomic number, symbol, name, atomic mass, etc.).
* Display chemical properties (electronegativity, electron configuration, oxidation states, etc.).
* Ability to search for elements by name, symbol, or atomic number.

1. Basic Calculations:

* Calculate molar mass of compounds based on their chemical formulas.
* Perform stoichiometric calculations (mole ratios, limiting reactants, etc.).
* Calculate simple properties like density, molarity, and volume.

1. Error Handling:
   * Validation of user input to prevent incorrect data entry.
   * Proper handling of exceptions and errors.
2. Data Storage and Retrieval:

* Store element data in a structured format (JSON, CSV, database, etc.).
* Efficient retrieval of data during computations.

1. Unit Conversion:

* Support for unit conversion (e.g., grams to moles, Celsius to Kelvin).
* Consistent units throughout calculations.

Non-Functional Requirements:

1. Performance:

* Fast response times for retrieving element data and performing computations.
* Efficient memory usage, especially when dealing with large datasets.

1. Scalability:

* Ability to easily add new features or extend existing ones.
* Scalable architecture to accommodate future enhancements.

1. Compatibility:

* Compatibility with major operating systems (Windows, macOS, Linux).
* Compatibility with different Python versions (e.g., Python 3.x).

1. Security:

* Secure handling of user input to prevent injection attacks.
* Data encryption if sensitive data is stored (e.g., user preferences).

1. Usability:

* Intuitive interface design for users with varying levels of expertise.
* Clear and concise documentation for users and developers.

1. Reliability:

* Minimal bugs and errors.
* Robust error handling to gracefully handle unexpected situations.

1. Maintainability:

* Well-structured code following best practices and coding standards.
* Adequate comments and documentation to facilitate maintenance by other developers.

1. Portability:

* Easy deployment on different systems without major modifications.
* Minimal dependencies on external libraries or resources.

## Out-of-scope

N/A

## Future Goals

1. Periodic Table Representation:

* Visual representation of the periodic table.
* Clickable elements for detailed information display.

1. User Interaction:

* User-friendly command-line interface or graphical user interface (GUI).
* Ability to input chemical formulas or equations.
* User prompts for input when necessary.

1. Compounds
2. Web Application

### Assumptions

N/A

# Solutions

## Existing Design

Web apps with links to various calculators. Cons: adds.

## Proposed Design