# Level 1 实验报告

姓名: 蓝俊玮 学号: PB20111689

实验环境: Windows 10 Python 3.9.0 Pycharm Community Edition 2021

### 1. 实验选题

Level 1.10 分子量计算:给定一个只含C, H, O, N的化学分子式,输出它的分子量

### 2. 实验思路

对于一个只含 C,H,O,N 的化学分子式而言,其化学分子式正确的格式一定是按  $C_xH_yO_mN_n$  来的,即每个数字之前一定会有一个字母,那么可以将每个元素单独提取出来,将输入的化学分子式进行分割,得到多个部分,然后计算出各部分总的质量,最后加起来便是化学分子式的质量。其中采用的方法是用正则表达式进行分割:

```
elements = re.findall('[A-Z][^A-Z]*', compound)
```

通过分割正则表达式分割,可以迅速且准确的得到各个原子的数量,同时还可以依此来判断输入的化学分子式是否有误(即判断输入了其他元素信息),当遇见错误时,则提示错误信息并返回重新输入。

### 3. 实验代码

```
import re
if __name__ == '__main__':
   element_lists = ['C', 'H', 'O', 'N']
   element_weight = {'C': 12, 'H': 1, 'O': 16, 'N': 14}
   error = False
   while True:
       compound = input('please input a chemical formula(quit or q to exit):
\n')
       if compound == 'quit' or compound == 'q':
           break
       compound = compound.upper() # 将输入的小写字母转化为大写字母
       elements = re.findall('[A-Z][^A-Z]*', compound) # 将四个元素分割开
       formula\_weight = 0
       for element in elements:
           if len(element) == 1:
                                 # 如果只有一个元素,没有数字时,即只有1个元素
              if element not in element_lists: # 如果输入了其他元素,则显示错误信
息
                  print("please input a correct chemical formula!")
                  error = True
              formula_weight = formula_weight + element_weight[element]
           else:
              if element[0] not in element_lists: # 如果输入了其他元素,则显示错误信
息
                  print("please input a correct chemical formula!")
                  error = True
                  break
```

```
formula_weight = formula_weight + element_weight[element[0]] *
int(element[1])
    if not error:
        print(formula_weight)
        error = False
    print("finishing calculated formula weight!")
```

## 4. 实验测试

在终端输入即可运行:

```
pip install -r requirements.txt
python level1.py
```

#### 当输入 $C_6H_6$ , $C_2H_4O_2$ , $C_2H_6ON$ 时:

```
"D:\PyCharm Community Edition 2021.1.3\python_homework\venv\Scripts\python.exe" "D:\PyCharm Community Edition 2021.1 .3/python_homework/Level1.py"

please input a chemical formula(quit or q to exit):

C6H6

78

please input a chemical formula(quit or q to exit):

C2H4O2

60

please input a chemical formula(quit or q to exit):

C2H6ON

60

please input a chemical formula(quit or q to exit):
```

#### 当输入错误分子式或退出信息时:

```
"D:\PyCharm Community Edition 2021.1.3\python_homework\venv\Scripts\python.exe" "D:\PyCharm Community Edition 2021.1 .3/python_homework/Level1.py"
please input a chemical formula(quit or q to exit):

C6H6
78
please input a chemical formula(quit or q to exit):

C7H8L9
please input a correct chemical formula!
please input a chemical formula(quit or q to exit):

q
finishing calculated formula weight!

进程已结束,退出代码为 0
```