NARSEE MONJEE EDUCATIONAL TRUST'S
JAMNABAI NARSEE SCHOOL
Narsee Monjee Bhavan, N. S. Road No. 7, J.V.P.D. Scheme,
Vile Parle (W), Mumbai - 400 049, India.
Tel.: +91-22-2618 7575 / 2618 7676 • Fax: +91-22-2614 6262
Website: www.jns.ac.in • e-mail: contactus@jns.ac.in

TO WHOMSOEVER IT MAY CONCERN

This is to certify that Khush Kothari of Jamnabai Narsee School- ISC Grade 12 has successfully completed the Chemistry project titled 'COMPUTATIONAL CHEMISTRY'.

The algorithm and program written to calculate the molecular mass of any given chemical compound is his original work and he has inferred the deductions successfully.

Pamela Castello

Ms. Pamela Castello
Teacher in Chemistry

JAMNABAI NARSEE SCHOOL MUMBAI 400 049

COMPUTATIONAL CHEMISTRY

1. AIM:
   To demonstrate the advantages of using computer softwares and programs in the field of chemistry and thus, create an efficient Java program to calculate and return the molecular mass of any chemical compound.

2. WHAT IS COMPUTATIONAL CHEMISTRY:
   Computational chemistry is a branch of chemistry that uses computer simulation to assist in solving chemical problems. It uses methods of theoretical chemistry, incorporated into efficient computer programs, to calculate the structures and the properties of molecules and solids.

3. PROCEDURE TO CREATE THE JAVA PROGRAM:
   - Write down the algorithm of the intended pogram.
   - Do the dry run to remove any logical errors that might be present.
   - Type the program on the BlueJ Application and compile it. Make sure there are no syntax errors.
   - Test the program with some sample inputs and verify the result manually.

4. ALGORITHM:
   - Start a class with the name Formula.
   - Declare two class variables, String chemform (to store the chemical formula) and double molmas (to store the molecular mass of the chemical compound).
   - In the parameterized constructor, initialize chemform with the user-input.
   - Create a function calculate(). Its purpose is to extract the elements from the compound and send it to another class called 'calculation'.
   - Initalize a string array of length=20.
   - Initialize a double massat variable to 0 and a double array,coeff, to store coefficient of the elements.
   - Initialize three integer variables a, i and end to zero.
   - Now begin the lexical analysis of your chemical compound.
   - Start a do-while loop.
   - Extract character using the charAt() function at index position i.
   - Now check if its uppercase.
   - If true, then store it in the string array and increment i by 1.
   - Repeat the process of extraction of the character.
   - Check if its lowercase. If true, store it in the string array at index position a and increment i by 1.
   - Thus, we will have our first element at the position a.
   - Then check if the next character is a digit.

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- If true, store it in the string coefficient and increment i by 1.
- The next character could again be a number, thus check again and if true, concatenate it with the previous coefficient and increment i by 1.
- Convert the string coefficient into double using valueOf() function.
- Increment a by 1.
- Put the test condition as i<=length of chemform-1.
- End the loop.
- Put end=a.
- Create an object obj of the class calculation and pass on value of end and the arrays s and coeff.
- Obtain mass of compound by calling a function mass() from class calculation.
- End function calculate().
- Create a function result() with return type double and return the variable molmas.
- Create the main() method.
- In the main(), create an object and call calculate() followed by result().
- Check if the value of the chemical compound exists or not and display the message accordingly.
- End class Formula.
- Start class calculation.
- Initalize two final double array variables, String symbol[ ] and double ma[ ], which will store all the existing element names and their masses respectively.
- Initialize class variable double masmol to 0.
- In the parameterized constructor, accept the arguments from the class formula. Search for the element and its mass in the arrays symbol and ma respectively.
- Add the product of mass and the coefficient of that element to the masmol variable.
- End constructor calculation().
- Create method double mass() which will return the value of masmol to the class Formula.
- End class calculation.

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ACKNOWLEDGEMENT

Computational Chemistry is a topic which involves the subjects, computer science and chemistry. I have chosen this topic as I wanted to learn about the applications of computer programming in solving chemical equations and numericals. It has been a great learning experience and as a result I have been able to create a Java Program which computes and displays the molecular mass of any chemical compound as inputted by the user.

I am thankful to and fortunate enough to get constant encouragement, support and guidance from all Teaching staff of Jamnabai Narsee School (My high school), which helped me in successfully completing my project work. Also, I would like to extend my sincere esteem to Mrs.Minu Joshi (Head of the ICT Department) and Mrs. Pamela Castello (Teacher, Department of Chemistry) for their timely support.

Getting through my project required more than academic support, and I have many, many people to thank for listening to and, at times, having to tolerate me over the past few months. To my parents and my sister– it would be an understatement to say that, as a family, we have experienced some highs and lows in the past few months. Every time I was ready to quit, you did not let me and I am forever grateful. This project stands as a testament to your unconditional love and encouragement.

Lastly, I hope to continue my work at college and hope that with the effective expertise and guidance of professors at college I shall gain a better appreciation towards the subject and embark on a journey of discovery.

Khush Kothari.

Pamela Castello