Welcome students
Program Bachelor of Science. Third year in the subject of chemistry, semester 5, paper code, CHC 105 paper title, physical chemistry,

title of the Unit Unit 2 Quantum Chemistry Module name. Mathematical concepts,derivatives and 2nd order derivatives, module number 22.

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Outline of this module, introduction to derivatives, rules of derivatives, derivatives of different functions, chain rule of derivatives, partial derivatives and higher order derivatives.

Learning outcomes. at the end of this module, the students will be able to understand the concept of derivative. Get familiar with the rules of derivatives and derivatives of common functions. The students will be also able to understand partial derivatives and higher order derivatives.

So what is a derivative? In mathematics, the derivative is defined as the rate of change of a function with respect to a variable. Derivatives are fundamental to the solution of problems in calculus and differentiale quations. If I have a function, Y is equal to F of X, then the derivative of this function at a point X is defined as. F dash of X is equal to limit as H tends to zero F of X+ H minus F of X whole divide by H. This equation is known as the first principle of derivatives. Now this equation can also be written as limit as Delta X tends to 0 Delta Y divided by Delta X which is equal to dY by DX, so derivative is nothing but the rate of change in dependent variable with respect to the change in independent variable.

The process of finding the derivative is known as differentiation. Geometrically,the derivative of a function can be interpreted as the slope of the graph of the function, or, to be more precise, as the slope of the tangent line at a point.

Now let us see some of the rules of the derivatives. If I have two functions U & V, both functions of X, then D by DX of U plus V is given as derivative of U with respect to X plus derivative of V with respect to X. If we want to find the derivative of the product of two functions U into V this derivative is given by U into derivative of V with respect to X plus V into derivative of U with respect to X. This rule is known as the product rule, next derivative of U / V is given by V into derivative of U with respect to X minus U into derivative of V with respect to X whole divided by V square. This rule is known as the quotient rule.

Next power rules for positive and negative integers. The derivative of X raised to N is given by N into X raised to N minus one. So here N is any positive or a negative integer, and X is a variable. Derivative of any constant is always equal to 0. If I have a constant which is multiplied to a function, then the derivative of this quantity is equal to the constant can be kept outside the derivative that is. C into DU by DX, this rule is known as the constant multiple rule.

Now let us see the derivatives of some common functions which are used in chemistry. First. Derivatives of exponential and logarithmic functions, derivative of an exponential function, e raised to X is e raised to X itself, derivative of A raised to X is equal to A raised to X into log of A. Here, A is a constant and X is the variable. Derivative of log X is equal to 1 upon X.

Next. Here I have listed the derivatives of some of the trigonometric functions. The most important of this trigonometric functions are the derivatives of sine X and the derivative of Cos X. Derivative of sine X is Cos X and the derivative of Cos X is minus of sine X. Similarly we have the derivative of tan X, cot x, sec x and cosec X. Now all these derivatives are derived from the first principle of derivatives

coming next to the chain rule of derivatives. The derivative of the composite of two differentiable functions is the. Product of their derivatives evaluated at appropriate points. So this derivative is given by dY by DX is equal to dY by DU into dU by DX. Now let us understand this concept by taking an example. So consider a function Y is equal to three X ^2 + 1 the whole square. Now this is an example of a composite function. This function can be written as Y is equal to U square where U is equal to three X ^2 + 1. So by using the chain rule I can differentiate Y with respect to X which is given by dY by DU into DU by DX. This is further equal to derivative of U square with respect to U into derivative of three X ^2 + 1 with respect to X. The derivative of U square with respect to U is 2 U and the derivative of three X ^2 + 1 with respect to X is 6 X. So on substitution of U I will get 2 into three X ^2 + 1 into 6X. So on further simplification I will get 36 X raised to 3 + 12 X

coming next to the partial derivatives. So if I consider a function Z which is a function of two variables X & Y, then I can differentiate this function Z with respect to X, keeping Y constant or. I can also differentiate this function Z with respect to Y keeping X constant. These derivatives are known as the partial derivatives. Let us consider an example. Consider Z is equal to X ^2 + 2 X y + y ^2. So I will differentiate this function Z with respect to X, keeping Y constant. So I will get partial derivative of Z with respect to X, keeping Y constant is equal to. Partial derivative of X square with respect to X plus. Now when I'm differentiating with respect to X i need to keep Y constant SO 2Y I can take it outside the derivative so I will get two Y into partial derivative of X with respect to X plus partial derivative of Y square with respect to X. Now the derivative of X square with respect to X is two X + 2 Y is constant partial derivative of X with respect to X is 1 plus derivative of Y square with respect to X will be equal to 0. So I will get partial derivative of Z with respect to X, keeping Y constant is equal to two X + 2Y. Similarly, we can find the partial derivative of a function Z with respect to Y, keeping X constant

coming next to the higher order derivatives. Higher order derivative means differentiating a function more than once. So if I differentiate a function once, it is known as. The 1st order derivative if I differentiate it 2 times, it is known as The 2nd order derivative and so on. So let us see an example. So consider a function Y is equal to sige of two X + 3. Now again this is a composite function, so its first derivative will be two into cos of two X + 3. So if I further differentiate this function with respect to X I will get the second derivative of it. second derivative with respect to X will be D2Y by DX Square will be equal to minus four sine of two X + 3.

So here are the references for this module,

thank you.