

# SCC 202 Lab Experiment 2

Inquiry and Problem Solving Competency, Writing, and Digital Ability

## Using Computational tools to find pKa values

### Pre-Requisites

SCC 201 Lab 7: Molecular Models, Lewis Structure and Molecular Geometry

SCC 201 Lab 8: Molecular Properties, Bond Length and VSEPR

SCC 201 Lab 9: Basic Computer Molecular Modeling using Gaussian: Molecular Energies

SCC 202 Lab 1: Gaussian Lab: Dipole Moments of Molecules

### Introduction

The term theoretical chemistry may be defined as the mathematical description of chemistry. Currently, there are two ways to approach theoretical chemistry problems: computational theoretical chemistry and non-computational theoretical chemistry.

Computational theoretical chemistry is primarily concerned with the numerical computation of molecular electronic structures and molecular interactions and non-computational quantum chemistry deals with the formulation of analytical expressions for the properties of molecules and their reactions.

The term computational chemistry is usually used when a mathematical method is sufficiently well developed that it can be automated for implementation on a computer. Computational chemistry is the application of chemical, mathematical and computing skills to the solution of interesting chemical problems. It uses computers to generate information such as properties of molecules or simulated experimental results. Very few aspects of chemistry can be computed exactly, but almost every aspect of chemistry has been described in a qualitative or approximate quantitative computational scheme. The biggest mistake that computational chemists can make is to assume that any computed number is exact. However, just as not all spectra are perfectly resolved, often a qualitative or approximate computation can give useful insight into chemistry if you understand what it tells you and what it doesn't.

Computational chemistry has become a useful way to investigate materials that are too difficult to find or too expensive to purchase. It also helps chemists make predictions before running the actual experiments so that they can be better prepared for making observations.

### Procedure:

1. Double click on the GaussView icon to open the program.

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