Introduction to Programming in Chemistry

LAB I

(1) Monte Carlo method of numerical integration for the calculation of pi. The students are asked to run this calculation and then to think of examples and discuss how this method might be useful in chemistry.

(2) Use Excel to find the inflection point in a pH curve (titration).

(3) Successive approximations. Write your own Excel code and use Excel to calculate $V$ in the van der Waals's equation of state

$$(P+n^2a/V^2)(V-nb)=nRT$$

using the method of successive approximations.

(4) Introduction to Spartan

LAB II

Using Excel:

(1) Do Excel Exercise 2.

(2) Do Excel Exercise 3.

(3) Do Excel Exercise 4.

Using Spartan:

(1) Computer lab on torsion angles in ethane and linear butane, and conformations of cyclohexane

(2) Computer lab on visualizing lone pairs, conformations of hydrazine, and resonance and inductive effects in basicity)