

Ollscoil na hÉireann, Gaillimh
National University of Ireland, Galway

AUTUMN EXAMINATIONS, 2002

THIRD SCIENCE EXAMINATION

CH314 CHEMINFORMATICS AND VALIDATION

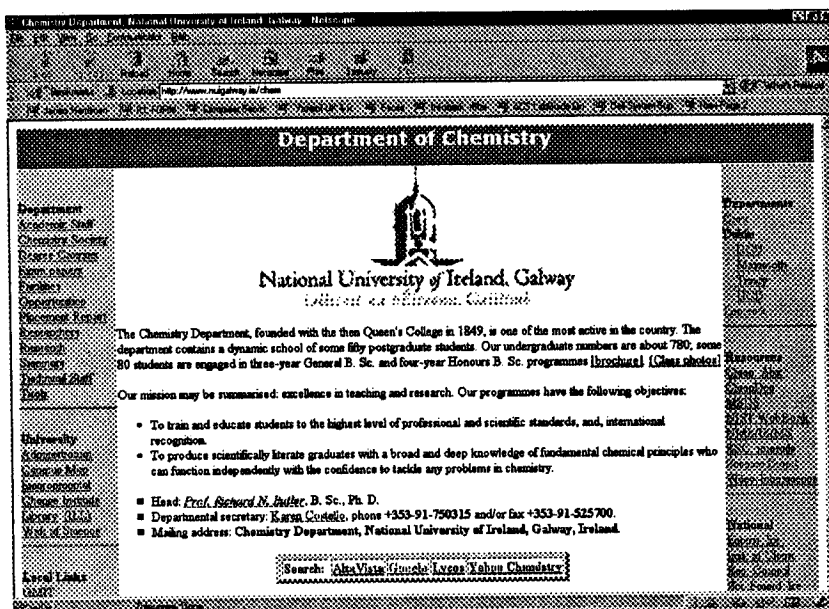
Professor J. Evans
 Professor R.N. Butler
 Professor M.J. Hynes
 Professor P. McArdle
 Dr. J. Simmie
 Dr. N.W.A. Geraghty

Time allowed: Two hours

Attempt **two** questions from each section
 Use separate answer books for Sections A and B
 Marks: All questions carry equal marks

Section A

- With reference to the Department of Chemistry web page, see Figure below, outline what you consider to be the most useful scientific aspects of using the Internet, and, outline the special problems encountered by chemists.



See larger
version
attached.

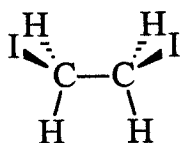
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2. Answer each of the following:

- (a) What are the names of the data bases that contain atomic coordinates derived from single crystal x-ray diffraction studies ? [4 marks]
- (b) If you were asked to provide atomic coordinates for a published molecular structure that had been determined by crystallographic methods, what criteria would you use to select suitable data ? [4 marks]
- (c) Is the information available from crystallographic data bases free ? [2 marks]
- (d) Name three important file formats used for atomic coordinate data. [3 marks]
- (e) When a file has been downloaded, what is the simplest way to tell if an atom coordinates are in fractional or Cartesian coordinates ? [4 marks]
- (f) What type of molecular orbital calculations are suitable for transition metal complexes ? Give a short explanation of your answer. [8 marks]

3. Answer each of the following;

- (a) Explain in general terms how the strain energy of a molecule is evaluated using molecular mechanics. [6 marks]
- (b) List the types of strain energy that are considered in a molecular mechanics calculation and indicate in detail how any **one** of them is computed. [6 marks]
- (c) Draw an energy/torsion angle plot for the following molecule based on the I-C-C-I torsion angle: [7 marks]



- (d) Label the global minimum and any one local maximum, and draw Newman projection formulae for the conformations corresponding to each. [6 marks]

4. Write notes on each of the following:

- (a) The concept of conformation. [7 marks]
- (b) Energy minimization / optimisation in molecular modelling. [6 marks]
- (c) Conformational searching. [6 marks]
- (d) Explain the difference between molecular mechanics and quantum mechanics based molecular modelling, outlining the advantages and disadvantages of each. [6 marks]

Turn over

Section B

5. Outline the procedures necessary to validate an analytical method for use in a pharmaceutical plant selling product into the U.S. [25 marks]
6. What is ISO 9000 ? Describe the steps that an organisation must take in order to secure accreditation for ISO 9000:2000. [25 marks]
7. What is process validation? Describe the key elements of process validation. [25 Marks]
8. Describe the steps involved in obtaining market authorisation from the FDA for a drug once it is discovered in the laboratory. [25 marks]