
SUMMER EXAMINATIONS, 2000

Third Science Examination

CH-314 Cheminformatics and Validation

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Dr. N. W. A. Geraghty
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Time allowed: Two hours

Attempt **two** questions from each section

Marks: All questions carry equal marks

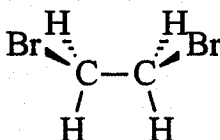
Section A

1. Answer **each** of the following

- (a) What type of information is on the CCD (Cambridge) data base ?
- (b) What methods are available for obtaining access to the CCD ?
- (c) What are the file formats in which data may be downloaded ?
- (d) Give the name of each of the following file formats:
.INS, .XR, .PDB and .CIF.
- (e) Which of the following is the most recent and comprehensive format:
.INS, .XR, .PDB and .CIF ?
- (f) What is the simplest way to tell if an atom coordinate file is in fractional or Cartesian coordinates ?
- (g) Explain clearly the reason why molecular mechanics is more difficult to apply to systems comprised entirely of elements other than C, H, N and O.
- (h) What type of molecular orbital calculations are best suited to transition metal complexes ?

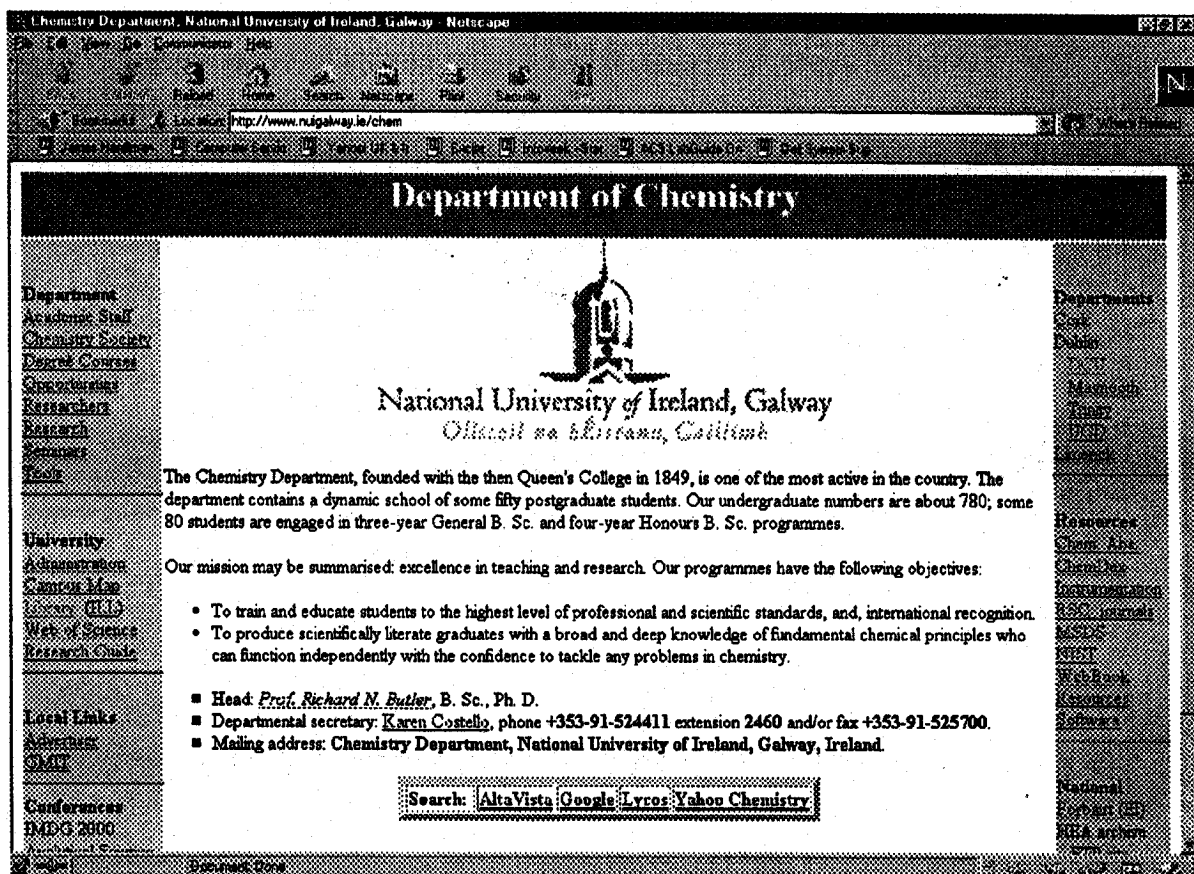
2. List the types of energy that are included in a molecular mechanics energy calculation and discuss in detail how any **three** of them are computed.

Draw an energy / torsion angle plot for the following molecule based on the Br-C-C-Br torsion angle.



Label the global minimum and the global maximum, and draw Newman projection formulae for the conformations corresponding to each.

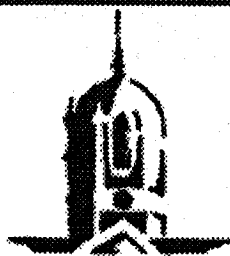
3. Write notes on each of the following:
- Conformational searching
 - Molecular dynamics
 - The application of molecular mechanics to any molecule or reaction of your choice.
 - Energy minimization / optimization
4. With reference to the Department of Chemistry web page, see Figure below, outline what you consider to be the most useful scientific aspects of using the Internet, and, outline the special problems encountered by chemists.



Section B

5. Outline the procedures necessary to validate an analytical method for use in a pharmaceutical plant selling product into the U.S.
6. Outline the procedures necessary to implement an effective cleaning protocol in a plant manufacturing active pharmaceutical ingredients (APIs).
7. Review the life cycle of the process for obtaining registration for a drug in the U.S. from laboratory synthesis to final registration.
8. Describe the PIC recommendations for the installation and operational qualification of equipment involved in the manufacture of pharmaceutical products.

Department of Chemistry



National University of Ireland, Galway
Ollscoil na hÉireann, Gaillimh

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The Chemistry Department, founded with the then Queen's College in 1849, is one of the most active in the country. The department contains a dynamic school of some fifty postgraduate students. Our undergraduate numbers are about 780; some 80 students are engaged in three-year General B. Sc. and four-year Honours B. Sc. programmes.

Our mission may be summarised: excellence in teaching and research. Our programmes have the following objectives:

- To train and educate students to the highest level of professional and scientific standards, and, international recognition.
 - To produce scientifically literate graduates with a broad and deep knowledge of fundamental chemical principles who can function independently with the confidence to tackle any problems in chemistry.
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