

Seminar

Monday 13 June 2011

11.00 am Room 531

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From antibiotics, via a jack-in-the-box, to SSED using GED –Structure (and acronyms) explained

When considering molecular structure, one instinctively thinks of a plot obtained from a crystallographer, which generally means that the structure was obtained in the solid phase. Whilst solid-state structure determination is ubiquitous in Chemistry Departments around the world, many industrial processes and chemical reactions actually take place in the liquid or gaseous phases, therefore provision for structure determination in these phases is vital. Using a technique called gas electron diffraction (GED) accurate gaseous molecular structures can be obtained. Valuable structural information is provided about molecules, free from the interactions that can affect solid-state structures.

This presentation will introduce the GED experimental method, the use of computational methods within the structure determination process, and discuss some pertinent examples. I will also explain what STRADAVARIUS, SARACEN, DYNAMITE, SEMTEX and SSED actually stand for, why they are important, and how they can be used to shape future research.