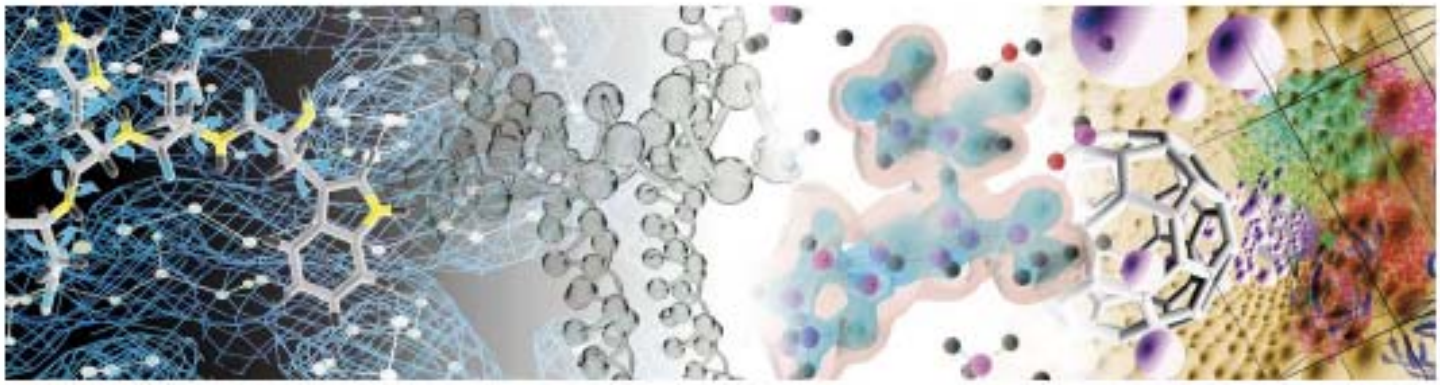
KEELE UNIVERSITY

Research Institute for the Environment, Physical Sciences & Applied Mathematics

CHEMICAL SCIENCES SEMINARS

PROGRAMME 2008

Lennard-Jones Laboratories 4pm LJ1.75



<u>Are Crystal Structure Predictable? A Challenge for Computational Chemistry</u>

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Given the chemical diagram of a molecule, is it possible to predict how it will crystallise (*i.e.* space group, unit cell parameters and all atomic coordinates)? The development of computational methods to address this problem has been a great challenge for computational chemistry over the past few decades and some methods are now starting to produce reliable predictions for simple systems. As the methods are further improved, and they become more generally applicable, the possibility of applying such calculations to the design of new materials with desired properties is becoming a reality. The presentation will describe recent developments and assessment of methods being developed for crystal structure prediction of organic molecules.