Curtin University

DEPARTMENT OF CHEMISTRY

SEMINAR SERIES

Pushing X-ray diffraction to the limit using "experimental" wavefunctions

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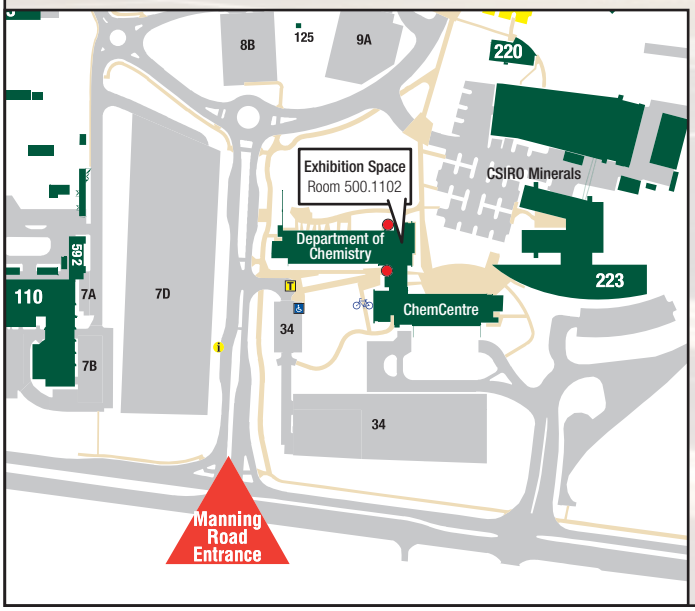
Our objective is to obtain the most accurate structural parameters and electron densities from X-ray experiments. The idea is to refine the parameters in a model wavefunction in order to fit the X-ray diffraction data. Two applications will be considered:

- First, we show that for a dipeptide, hydrogen atom positions and ellipsoids can be obtained in agreement with neutron diffraction measurements. This is the first time it has been done, quantitatively, and was thought to be impossible.

- Second, I will report on the ability to obtain accurate anharmonic vibration parameters for a drug-like molecule YQ28. Such information can be used to obtain the effective potential of mean force for the atom concerned. Obtaining anharmonic constants reliably was thought to be impossible due to model cross contamination between the bonding-electron and atomic displacement parameters. The electron densities obtained are about an order of magnitude more accurate than obtained before, without any special improvements in data measurement.



Friday, 18th October 2013 at 4:00 PM
Exhibition Space, Building 500, Room 1102

For more details about the Chemistry Seminar Series, please contact:

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