Mathematical Models for Computational Chemistry
Coordinate and Parameter Transformations

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Computational chemistry allows Synthesists to theoretically determine the 3-Dimensional structure of molecules relative to their minimum potential energy, in other words, their most stable configuration. The Force Field Method is one of many standard models that describes the energy of the molecule in terms of all the interactions that occur within the system of atoms, including stretching, bending, torsional, van der Waals, electrostatic and others. A stable molecular conformation can be found by minimising total energy function.

If there are N nuclei, then $3N$-6 coordinates define the molecule's geometry. As N increases, the number of local minima of the total energy grows exponentially with N. This consequently creates difficulties as numerical solution methods may become trapped in local minima. A computer program may have trouble distinguishing whether the molecular conformation exists in the natural world.

The search space for a suitable solution is greatly reduced when NMR Spectroscopy data is incorporated with the minimisation of the potential energy function. The power of having distance constraints between non-bonded atoms restricts the search space. The potential energy function can be expressed in the reduced dihedral angles space (internal coordinates). When a computer searches for absolute minimum, there will be limited variables to vary. I this project I understood the features and limitations of Force Field Methods.

I studied transformation of internal coordinates based on bond lengths, bending and dihedral angles to Cartesian coordinates. For a chain of four of atoms I obtained explicit formulas relating the internal coordinates with the distance between non-bonded atoms 1 and 4. Then I was able to convert the bounds on that distance (from NMR Spectroscopy) to the bounds on the dihedral angle, and hence reduce the search space. The same approach is applicable to longer chains of atoms. This would help compute stable conformations quicker.

Adela received an AMSI Vacation Scholarship in December 2008
See: www.ice-em.org.au/vs09.html

Studying coordinate and parameter transformations for the 2008-2009 Vacation Scholarship has enhanced my ability to overcome challenging tasks. The benefits of this project have highlighted the capability of reducing the amount of parameters required for mapping the positions of atoms in space. This will lead me into further investigation when I commence my honours. I would like to thank AMSI for this invaluable learning experience.

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