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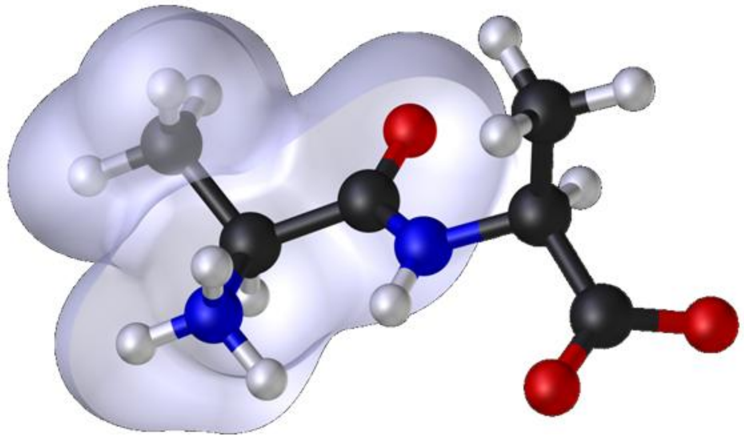
Why do computational chemistry?



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Lab work vs *in silico*

vs

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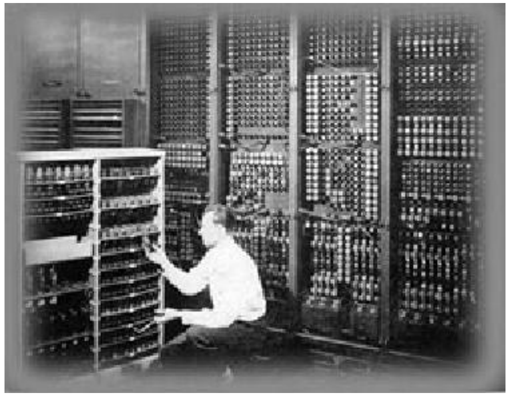
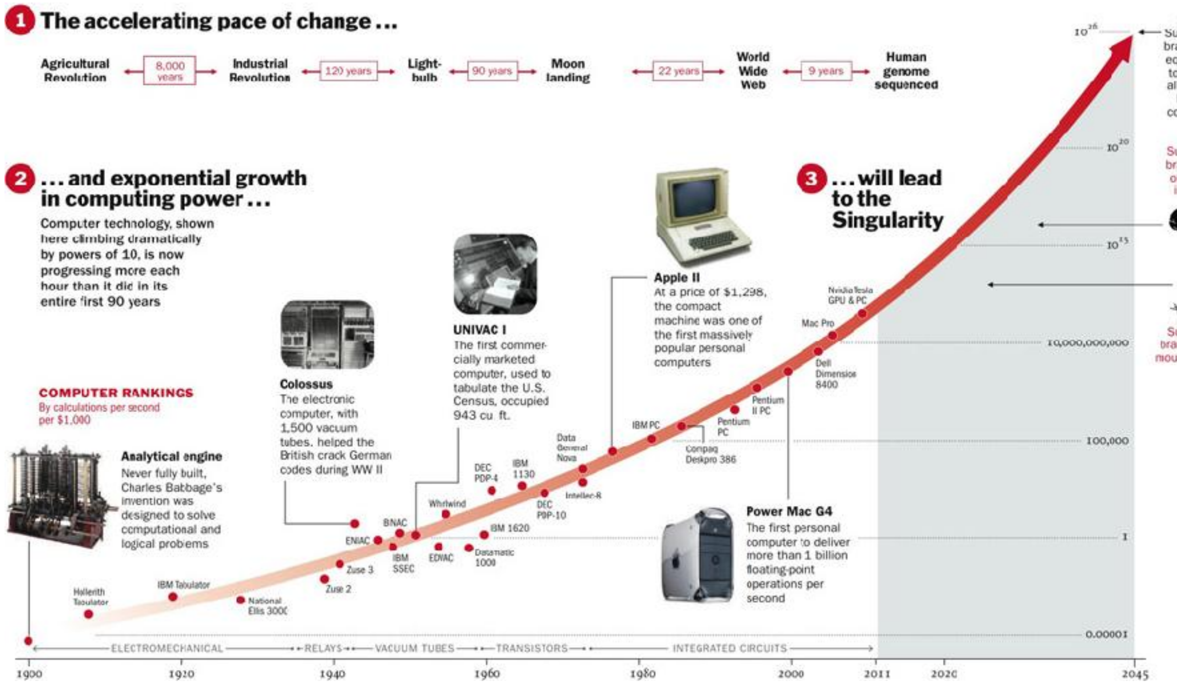
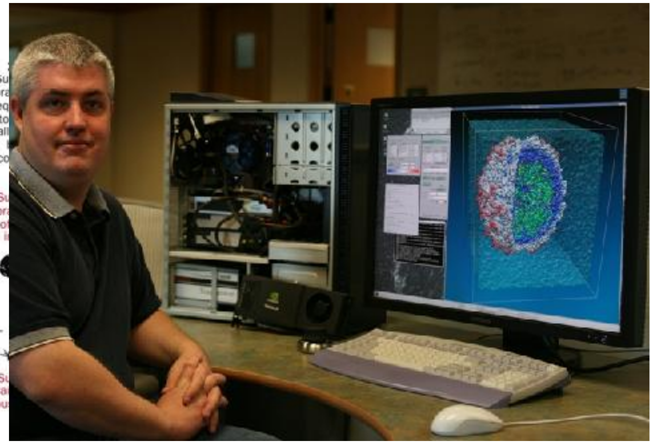
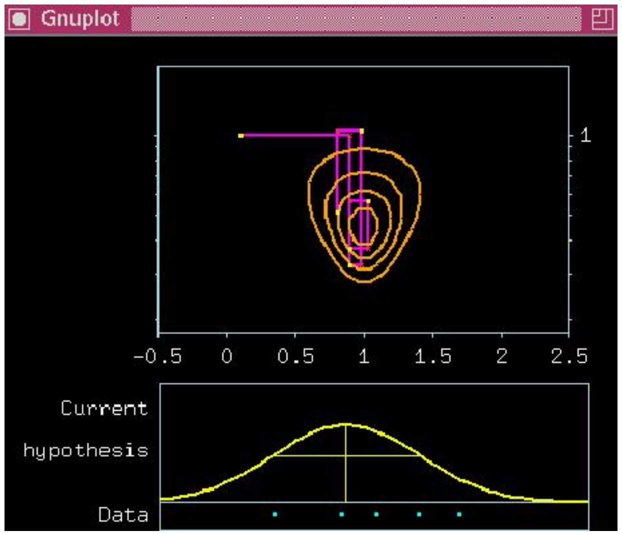
Evolution of computational chemistry

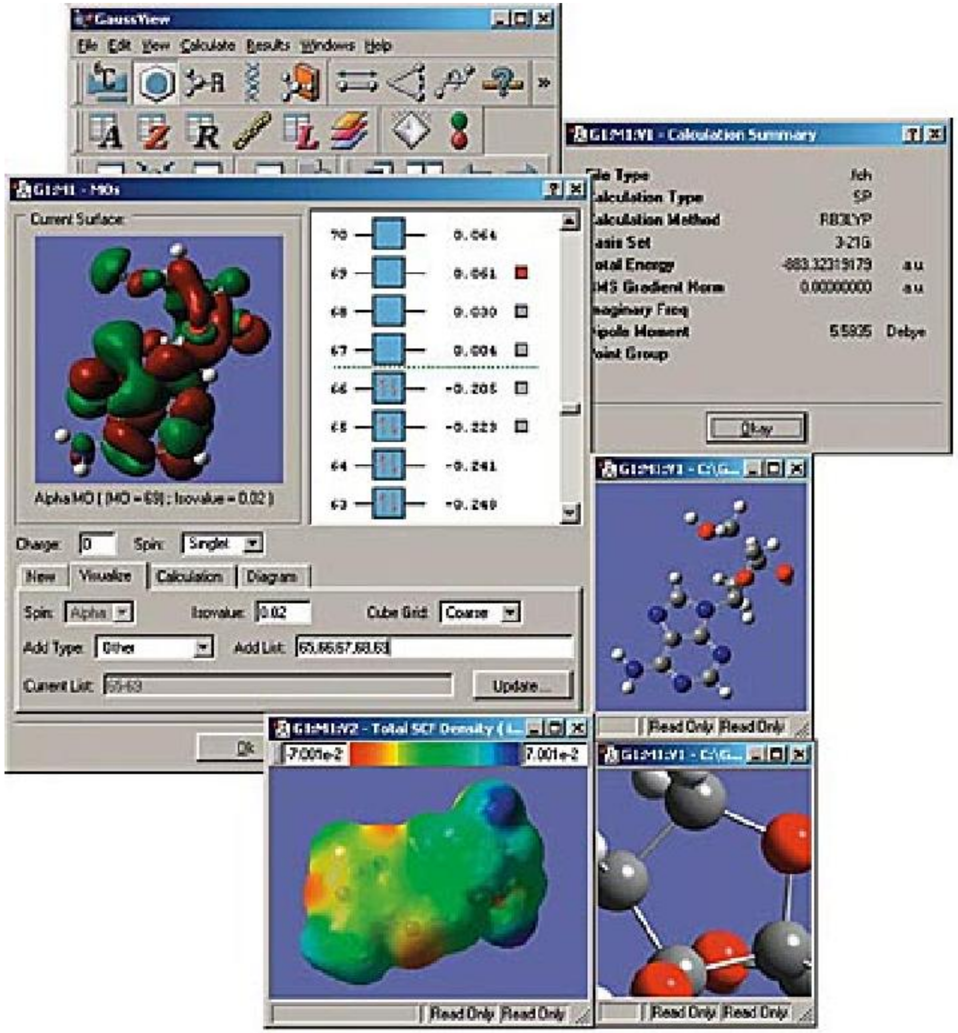






Evolution of computational chemistry





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What computational chemistry brings

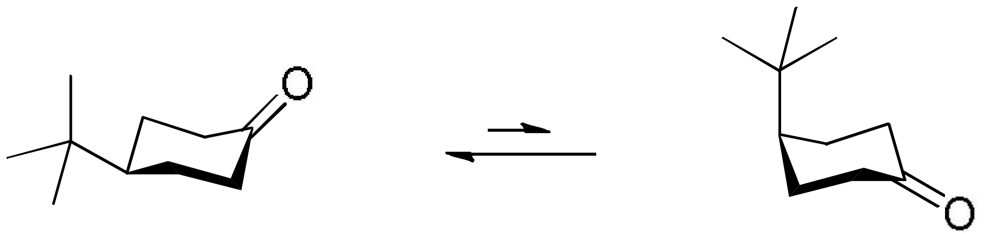
Computational chemistry can

- Explains chemical behaviours which might not be obvious to our chemical intuition.
- Predicts chemical behaviours from molecular properties and stability to reactivity and selectivity.
- Give us direct access to species which are not possible to observe with any physical or chemical techniques, i.e. transition states.

Some examples

- Energy minimisation and molecule visualisation, leading to insights about reactivity and stereocontrol.

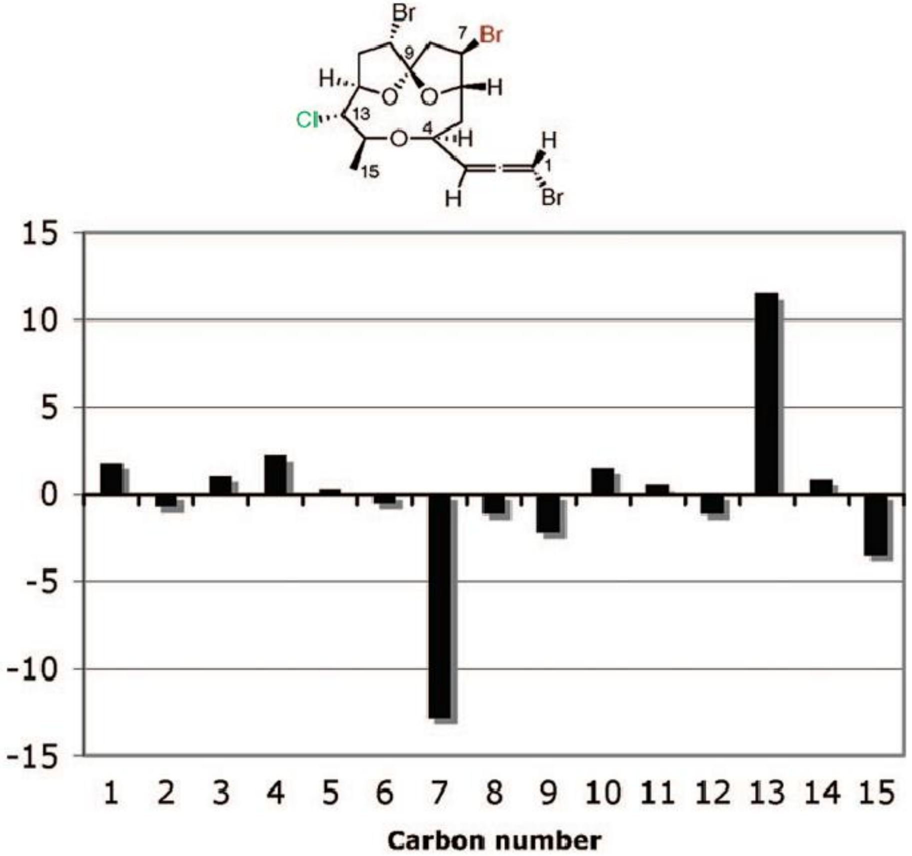
- Comparison of energies of isomers of starting material/product can help understand and predict reaction outcomes.

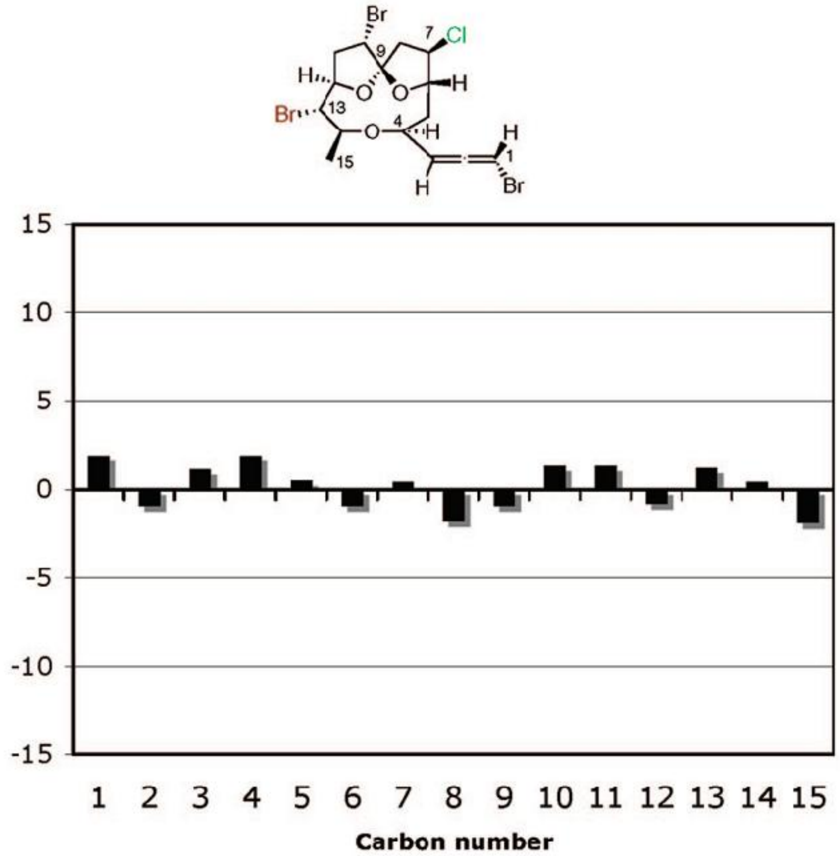


ΔE ⟶ Equilibrium constant K

Some examples

- Spectroscopic prediction can help assignment of complex molecules.





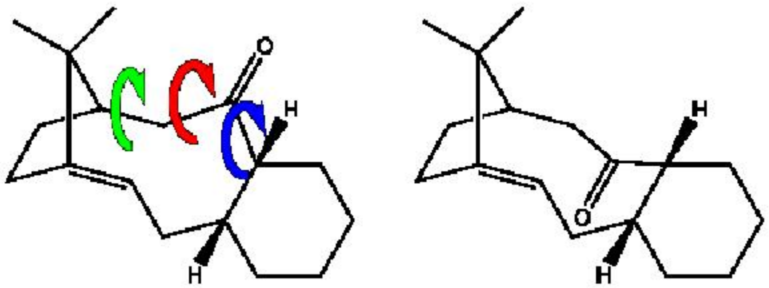
Rzepa and Braddock, *J. Nat. Prod.* **2008**, *71*, 728.

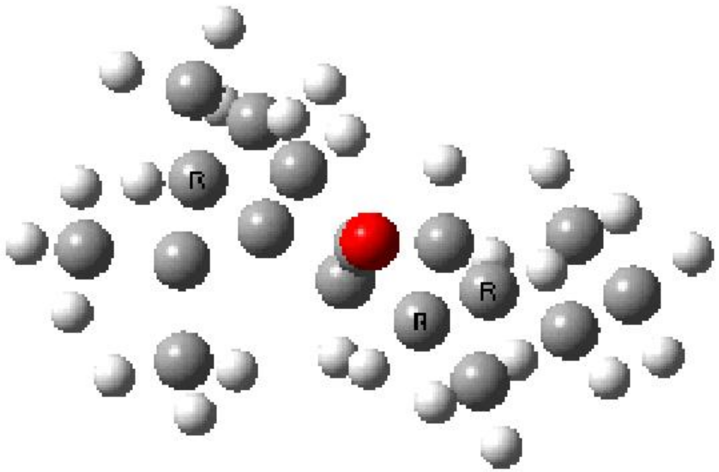
Some examples

- Molecular orbital calculations allow determination of their energy levels and visualisation of key orbitals to improve our understanding of bonding and reactivity (HOMO and LUMO).

  http://www.chemtube3d.com/Cycloaddition2.html

- Transition state modelling





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The course structure

- Module 1: Structure and Spectroscopy

  - Problems
  - Mini project

- Module 2: Bonding

  - Problems
  - Mini project

- Module 3: Transition States and Reactivity

  - Problems