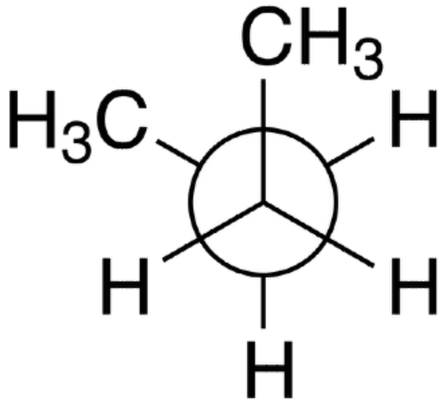
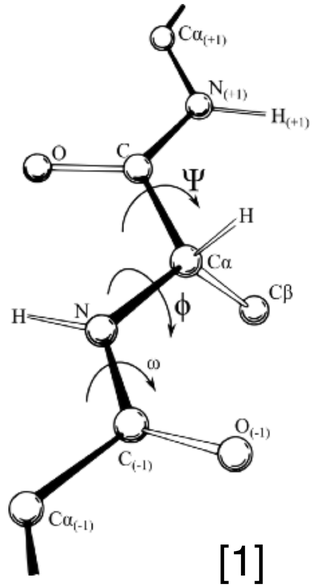
Dimensionality reduction with principal component analysis

Dimensionality reduction

- Biomolecular simulations have 3N dimensions, but in practice, functionally relevant macromolecular motion can be described with a lot fewer.
- Cartesian coordinates (x, y, and z) of each atom are the most common description but molecular systems can be described by other coordinate systems
- You have probably already seen
  - the free energy of butane as a function of the dihedral angle
  - the Ramachandran diagram, where protein backbones are described by the ϕ and ψ angles





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