LEARN FROM THEORY, EMPIRICAL OBSERVATIONS & EXPERIMENTAL DATA

First Principles

\[ E + hv = h \nu \]

\[ \Psi = \frac{1}{\sqrt{2}} \left( | \uparrow \rangle - | \downarrow \rangle \right) \]

\[ H_{\text{H}} \Psi = E \Psi \]

NMR CALCULATION & PREDICTOR METHODS

*Ab Initio*: Gauge-Including Atomic Orbital Method (GIAO)

ACD/Labs NMR Predictors

- Hierarchical Organization of Spherical Environments (HOSE)
- Artificial Neural Network (ANN)

STUDENT EXERCISE AT THE UNIVERSITY OF WATERLOO

GAUSSIAN Calculations

Hartree-Fock (HF)
Density Functional Theory (DFT)
Second order Møller-Plesset perturbation theory (MP2)
Basis Set: 6-31G(d)

ACD/Labs C+H NMR Predictors

HIGHLIGHTED RESULTS

Shielding Tensor Visualization

GAUSSIAN Calculations vs Experimental

ACD/Labs C+H NMR Prediction vs Experimental