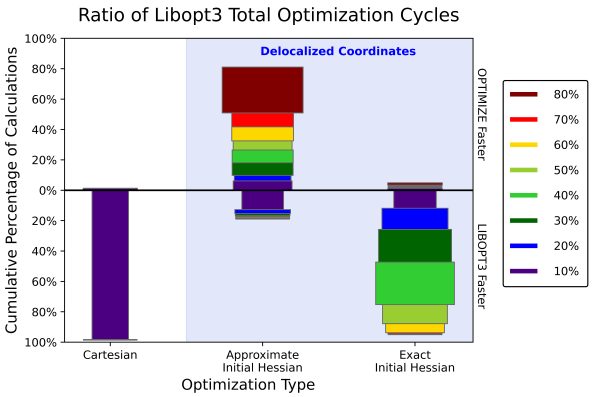
Q-CHEM™
A Quantum Leap Into the Future of Chemistry

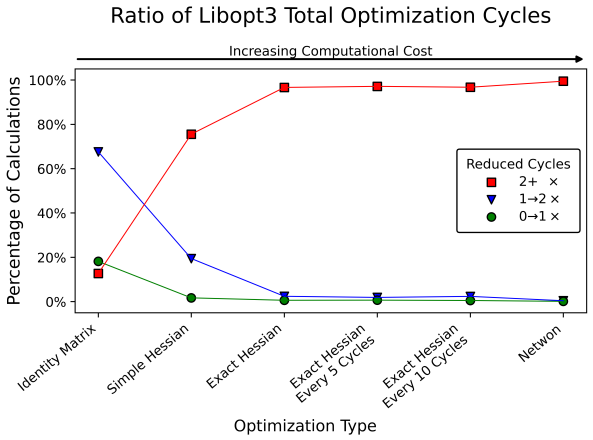
Modern Geometry Optimizer Driver: LIBOPT3

We are pleased to present a new modernized geometry optimization driver in Q-Chem for computing ground and excited state minima. This optimizer requires fewer total optimization cycles and gives users more control over the optimization algorithm, providing significant improvements in terms of flexibility and efficiency.

- Optimization Coordinates:
  - Cartesian
  - Redundant Internal
  - Delocalized Natural Internal
- Optimization Algorithms:
  - Gradient Based:
    - Steepest Descent
    - Conjugate Gradient
  - Exact Newton
  - Quasi-Newton:
    - BFGS
    - L-BFGS
    - Bofill
    - SR1
    - Powell-symmetric-Broyden
    - Farkas-Schlegel
- Recomputable Hessian for Quasi-Newton methods



A) Comparison of new LIBOPT3 driver to previous OPTIMIZE driver.



B) Comparison of the various Hessian controlability with respect to Cartesian optimization with LIBOPT3.

Request a free trial at www.q-chem.com