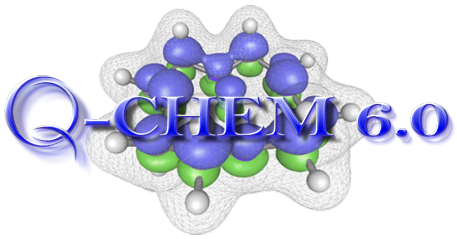
Q-CHEM™
A Quantum Leap Into the Future of Chemistry

Q-Chem 6.0 Features

We are pleased to present the sixth major release of the Q-Chem *ab inito* quantum chemistry software package, Q-Chem 6.0. Highlights in our new package include:

- Next-generation interface with external tools (generation of archive files in the HDF5 format)
- New geometry optimizer for ground and excited state calculations
- Analytic frequency calculations and orbital Hessians with the VV10 functional (Jiashu Liang)
- Developments in the nuclear-electronic orbital (NEO) family of methods, including NEO-CCSD and analytical gradients and Hessians for NEO-TDDFT (Zhen (Coraline) Tao, Patrick E. Schneider, Fabijan Pavosevic, Sharon Hammes-Schiffer)
- CCSD optical rotation evaluation (Josefine Andersen, Kaushik Nanda)
- Projection-based embedding with complex basis functions (Valentina Parravicini, Thomas Jagau)
- Complex-valued CC2, RI-CC2, and RI-CCSD (Cansu Utku, Garrette Paran, Thomas Jagau)
- EOM oscillator strengths in velocity and mixed gauges (Josefine Andersen, Sonia Coriani)
- Pairwise fragment excitation energy decomposition analysis (EDA) in QM/EFP calculations (Lyudmila Slipchenko)
- ...and many more! Visit the release log on our website for a full list.



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