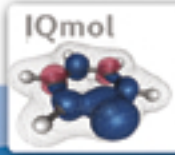
Q-CHEM™
A Quantum Leap Into the Future of Chemistry

New Release!
Q-Chem 4.0

We invite you to try our newest release, Q-Chem 4.0.

Q-Chem is a comprehensive ab initio quantum chemistry package for accurate predictions of molecular structures, reactivities, and vibrational, electronic and NMR spectra. The new release of Q-Chem 4.0 represents the state-of-the-art of methodology from the highest performance DFT/HF calculations to high level post-HF correlation methods.

Q-Chem is available stand-alone or as the fully integrated back-end of Spartan.



NOW AVAILABLE: iQmol, a free GUI which is downloadable at www.iqmol.org

www.q-chem.com

Sign up now to receive a Free 60-day trial of Q-Chem 4.0

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

FREE 60-DAY TRIAL

New Features Introduced in Q-Chem 4.0:

- Dispersion-corrected and double hybrid DFT functionals
- Faster algorithms for DFT, HF and coupled-cluster calculations
- Structures and vibrations of excited states with TD-DFT
- Methods for mapping complicated potential energy surfaces
- Efficient valence space models for strong correlation
- More choices for excited states, solvation and charge-transfer
- Effective Fragment Potential and QM/MM for large systems
- Shared-memory for multicores and implementations for GPU's

. . . and much more. Visit us at www.q-chem.com for a complete list of features.

www.q-chem.com