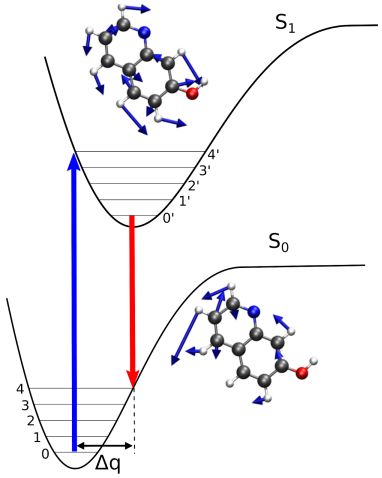
Q-CHEM™
A Quantum Leap Into the Future of Chemistry

Excited-State Properties from Analytic TDDFT Hessians

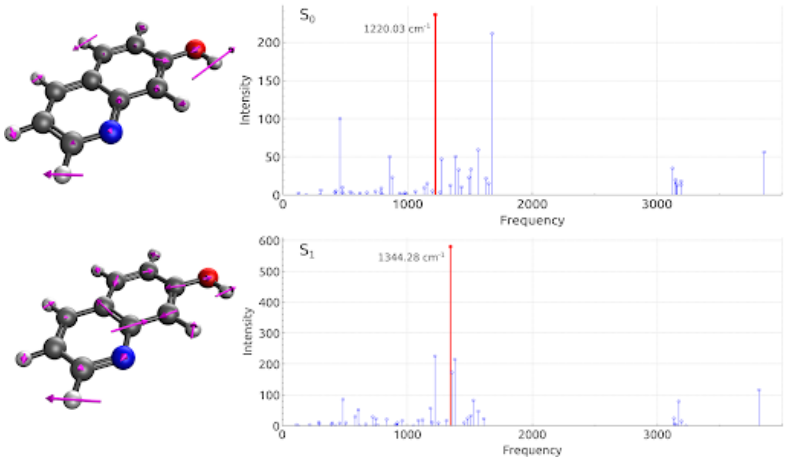
Analytic TDDFT Hessians are available for a wide range of modern exchange-correlation functionals including meta-GGAs:

- Much less costly than post-HF methods such as CASSCF and CC and thus applicable to larger molecules.
- Analytic Hessians are more efficient than numerical derivatives in geometry optimization. Excited-state geometry optimization can be more robust.
- Searching for critical points on excited-state potential surfaces is more robust with analytic Hessians.



Applications involving TDDFT Hessian calculations:

- Excited-state geometry optimizations and potential energy scans.
- Excited-state frequency calculations, time-resolved IR analysis.
- Fluorescence and phosphorescence, photochemistry and photophysics.
- Vibrationally resolved electronic spectroscopy simulation.
- Resonance Raman spectroscopy simulation.



Excited-state frequency analysis with meta-GGA xc functional MN15-L

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