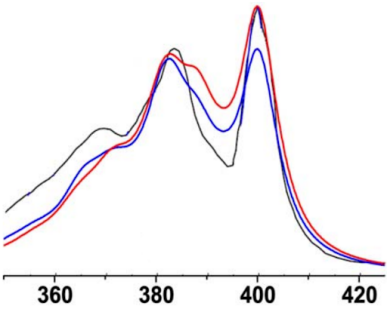
Q-CHEM™
A Quantum Leap Into the Future of Chemistry

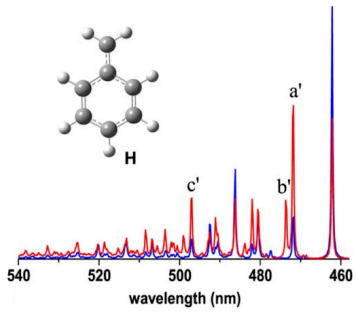
Simulating Vibrationally Resolved Electronic and Raman Spectra

A built-in module for computing vibrational progressions affords calculations of vibrationally resolved one-photon absorption (OPA), one-photon emission (OPE), and resonance Raman spectra (RRS):

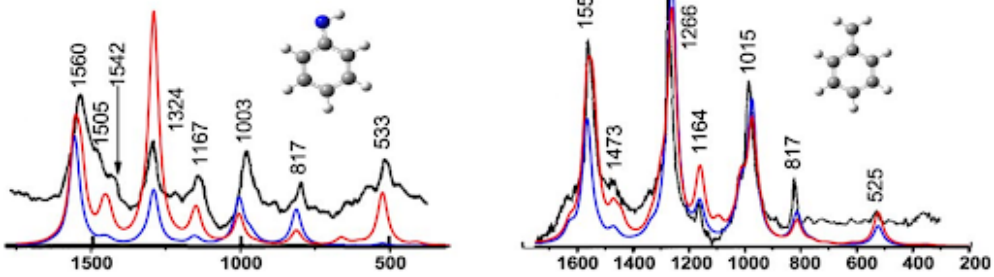
- Effective algorithm reduces computational costs by recasting sum-over-state expressions into the time-domain, thus avoiding explicit calculation of individual excited states.
- Different levels of theoretical treatment are implemented:
  - Franck-Condon (FC): includes only the zero-order term of the transition dipole moment.
  - Franck-Condon-Herzberg-Teller (FCHT): includes the zero- and first-order terms of the transition dipole moment.
  - Vertical gradient (VG): the excited state potential energy surface is approximated by a shift to the ground-state surface.
  - Duschinsky rotation: includes mode mixing effect.



(a) Calculated FC (blue) and FCHT (red) absorption spectra of $D_0 \rightarrow D_3$ transition for phenoxyl radical



(b) Calculated FC (blue) and FCHT (red) emission spectra of $D_1 \rightarrow D_0$ transition for benzyl radical



(c) Calculated FC (blue) and FCHT (red) RRS spectra for of $D_0 \rightarrow D_3$ transition for anilino (left) and benzyl (right) radicals.

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