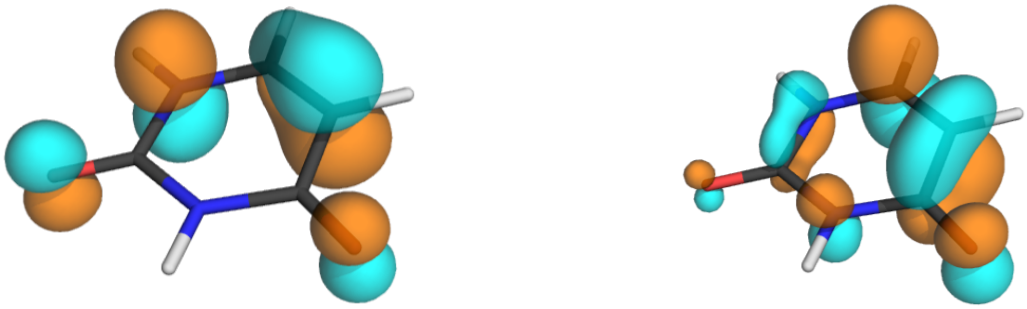
Q-CHEM™
A Quantum Leap Into the Future of Chemistry

Analysis of Excited-state Wave Functions

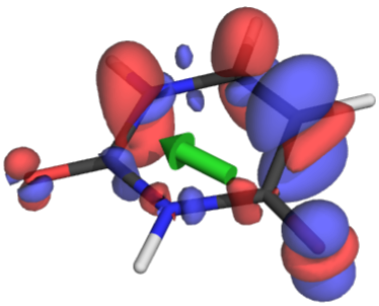
An extended wave-function analysis toolbox enables visualization of the excited states, automatic assignment of their properties, comparisons among different computational methods, and deeper insight into the underlying physics.



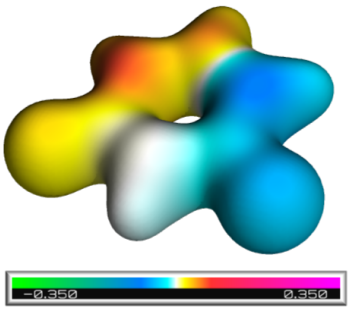
Hole and particle NTOs for the lowest bright excited state of uracil

Features include:

- Natural transition orbitals (NTOs) and attachment-detachment densities for a compact visualization of electronic transitions;
- Statistical analysis of spatial distributions to identify charge-transfer and Rydberg states;
- Transferability among various computational methods (ADC, EOM-CC, TDDFT) for benchmarking excited-state calculations;
- Computation of various electrostatic potentials to visualize energetic contributions to the excitation;
- Extension to molecular properties, non-linear spectroscopies, and resonances;
- Interface with the TheoDORE program for automatic state assignment and extended plotting capabilities.



(a) Transition density and transition dipole moment



(b) Electrostatic potential of the transition density, responsible for exchange splitting

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