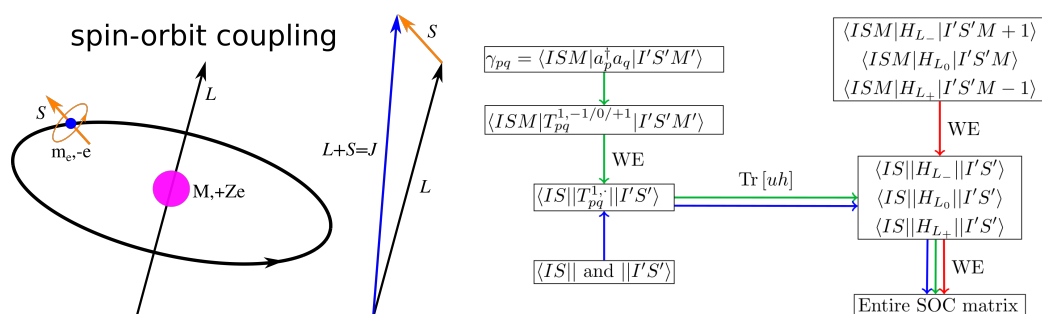
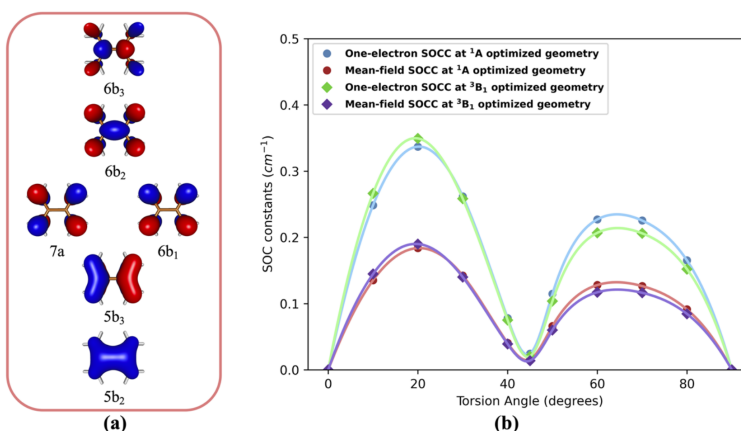


Calculating Spin-orbit Coupling with Q-Chem



- Different spin states mix up through spin-orbit coupling (SOC), thus it is essential to determine SOC to describe spin-forbidden processes, such as phosphorescence, intersystem crossing and spin-crossover, as well as magnetic properties;
- Q-Chem can calculate SOC at different levels of non-relativistic theory: a) CIS(TDA)/RPA(TDDFT); b) restricted active space configuration interaction (RASC); c) equation-of-motion coupled cluster (EOM-CC);
- The one-electron SOC can be evaluated using the one-electron Breit-Pauli operator or scaled nuclear charges;
- The full SOC can be evaluated using a mean-field treatment of the 2-electron part of the Breit-Pauli operator;
- All methods for SOC calculations can be combined with spin-flip excitations;
- Tools for visualizing SOC natural transition orbitals are available.



(a) π orbitals of tetramethylethane obtained from the ROHF septet reference on the ³B₁ optimized geometry with a zero torsion angle. (b) One-electron and mean-field SOC constants (SOCC) along torsion angles calculated for the two optimized geometries.