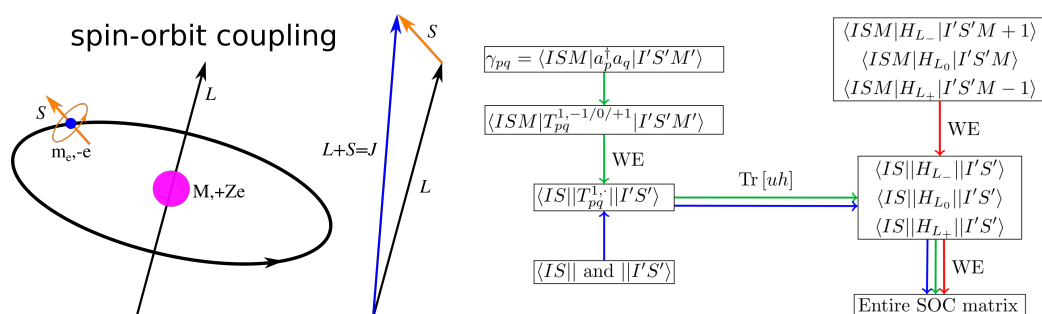# Q-CHEM™
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- The full SOC can be evaluated using a mean-field treatment of the 2-electron part of the Breit-Pauli operator;

- All methods for SOC calculations can be combined with spin-flip excitations;

- Tools for visualizing SOC natural transition orbitals are available.
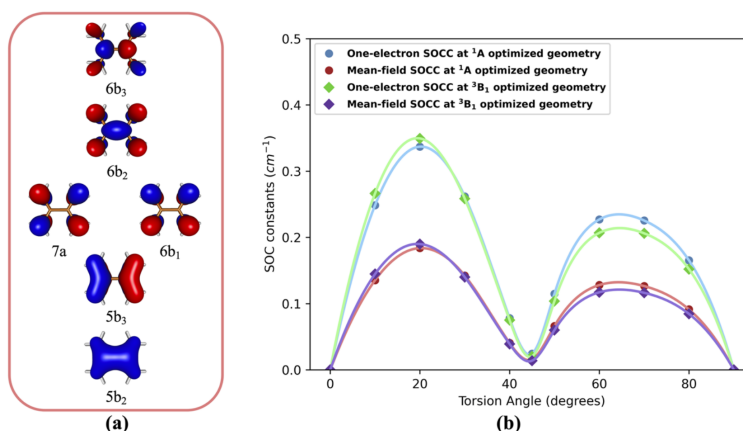
(a) π orbitals of tetramethyleneethane obtained from the ROHF septet reference on the $^3B_1$ optimized geometry with a zero torsion angle. (b) One-electron and mean-field SOC constants (SOCC) along torsion angles calculated for the two optimized geometries.

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