# Theoretical Modeling of the Core-Excited Spectrum of Benzyne Diradicals

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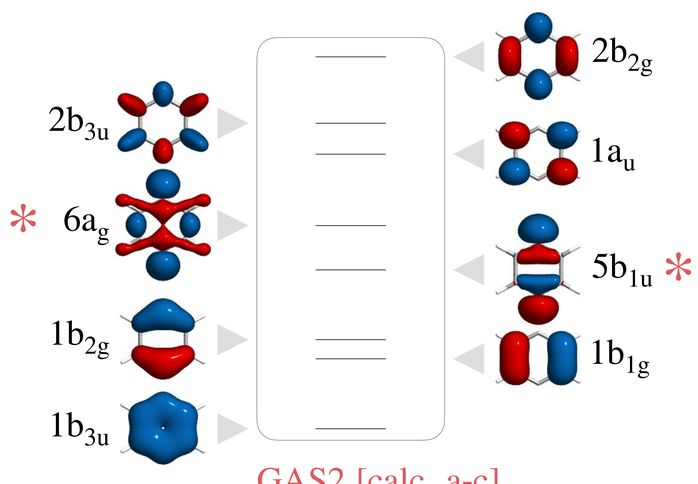
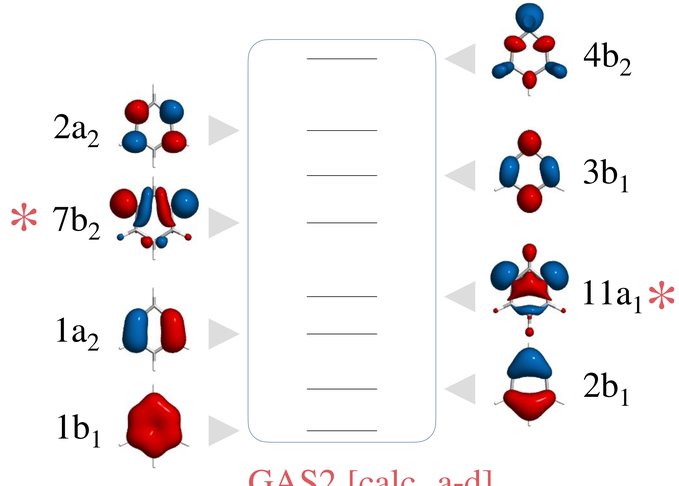
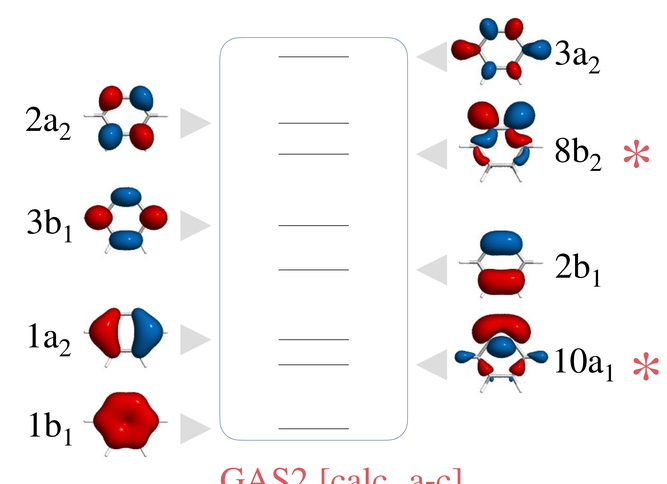
## S1 Active Spaces for GASSCF($N_{val}$ +1 e, $N_{val}$ o; $N_{core}$ -1 e, $N_{core}$ o) Calculations




*para*-benzyne




*meta*-benzyne




*ortho*-benzyne

✻ Orbitals included in GAS1 of GASSCF(3e, 2o; 3e, 2o) calculation.

✻ Orbitals included in GAS2 of GASSCF(3e, 2o; 3e, 2o) calculation.