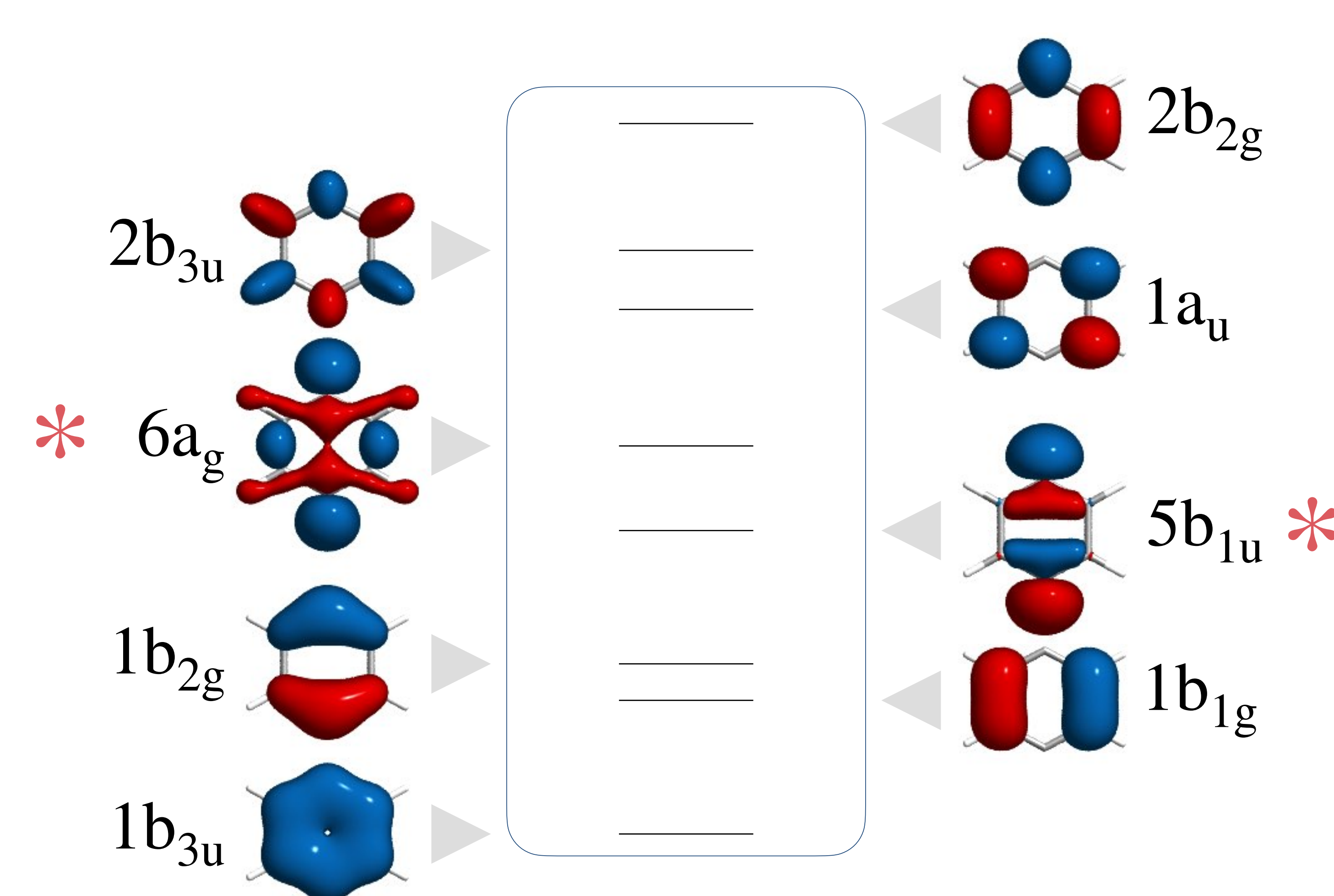
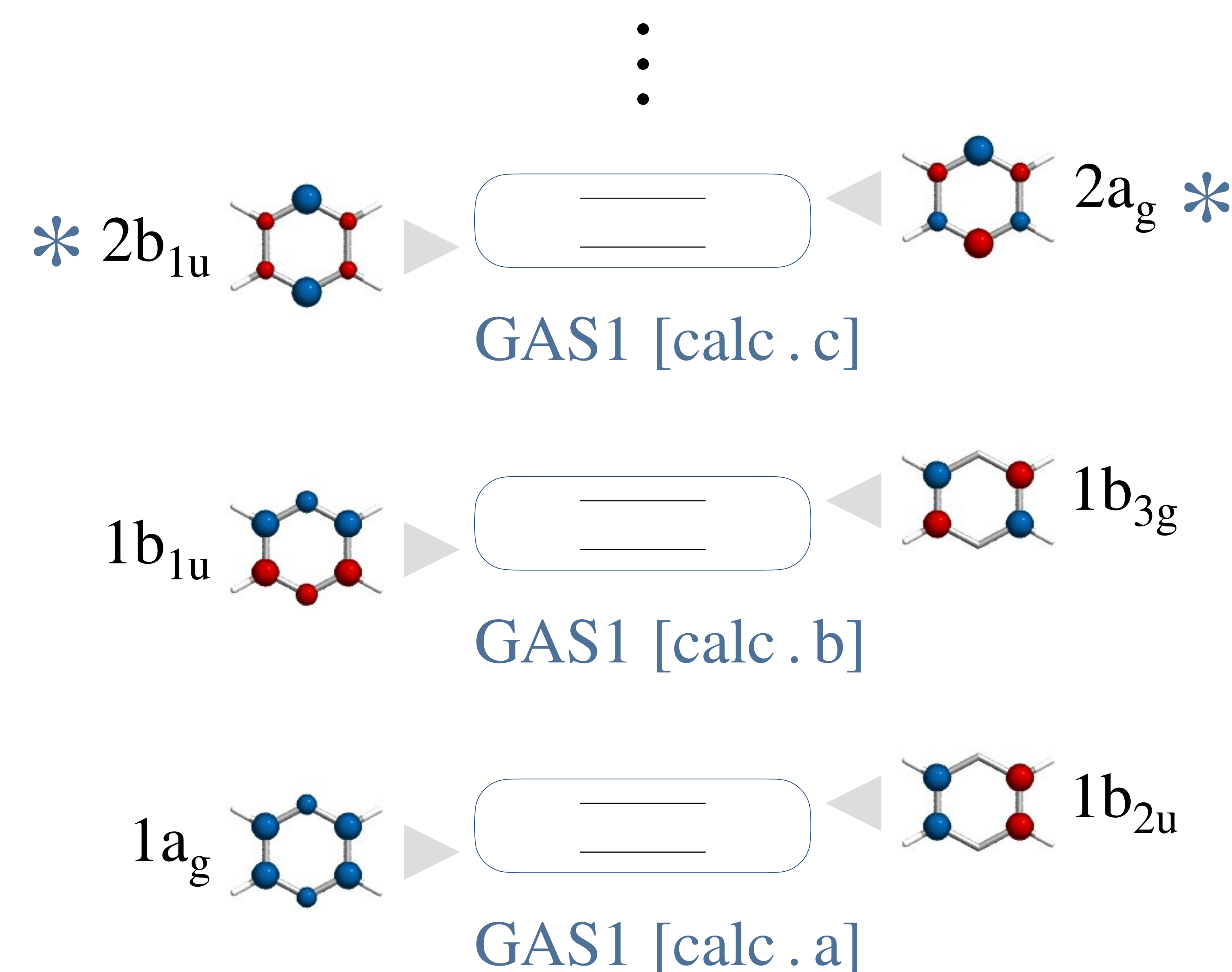




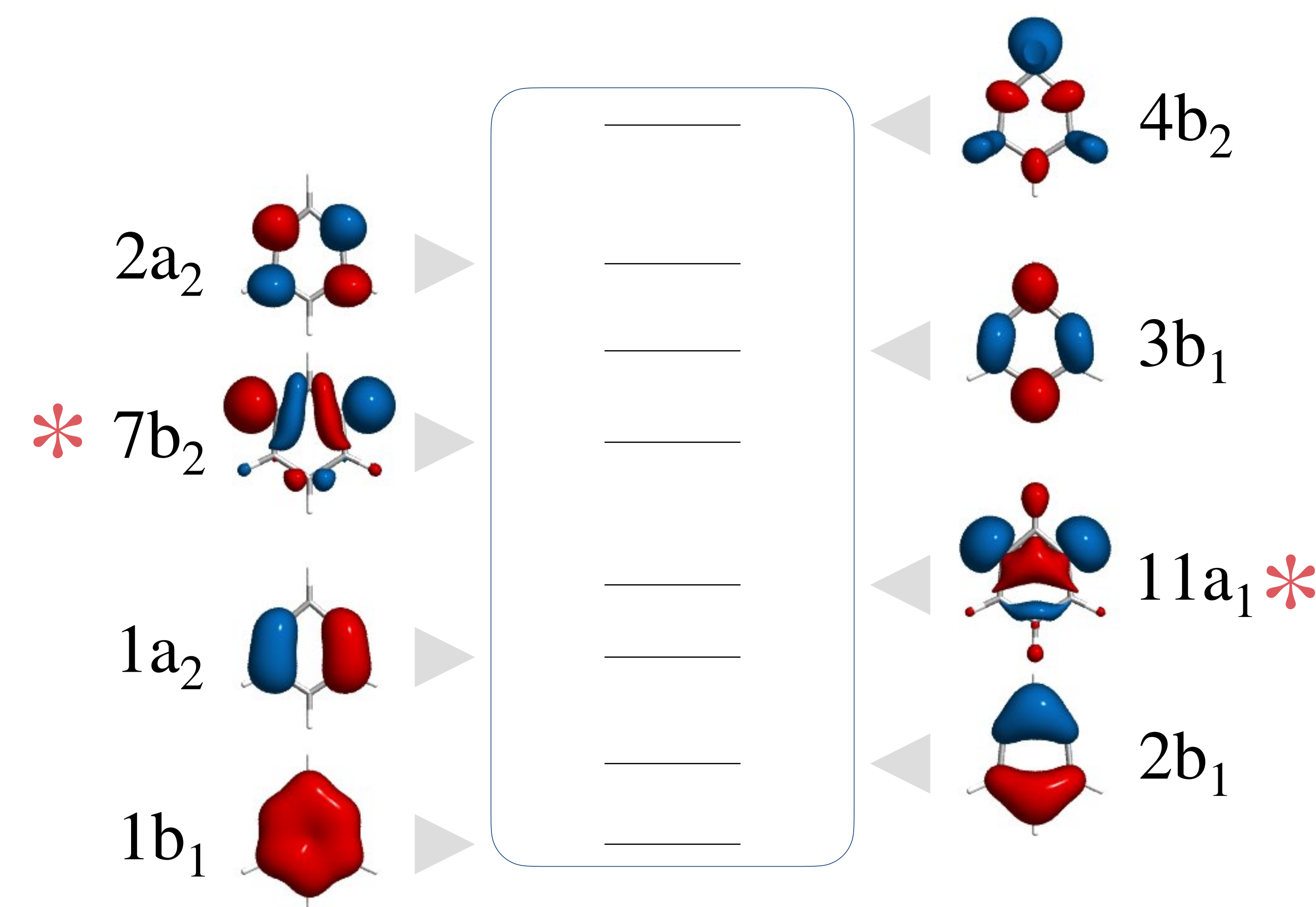
S1 Active Spaces for GASSCF($N_{\text{val}} + 1$ e, N_{val} o; $N_{\text{core}} - 1$ e, N_{core} o) Calculations



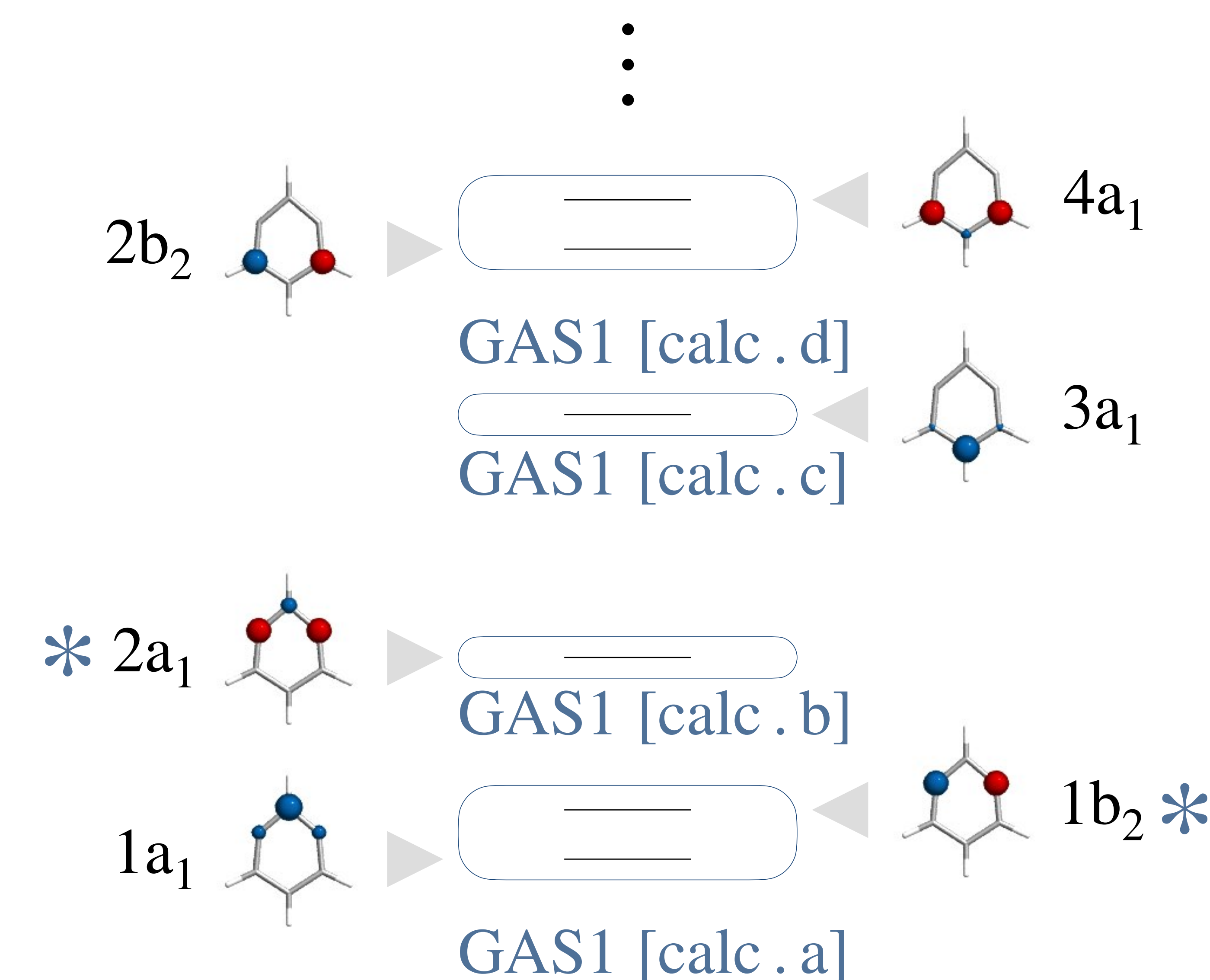
GAS2 [calc . a-c]



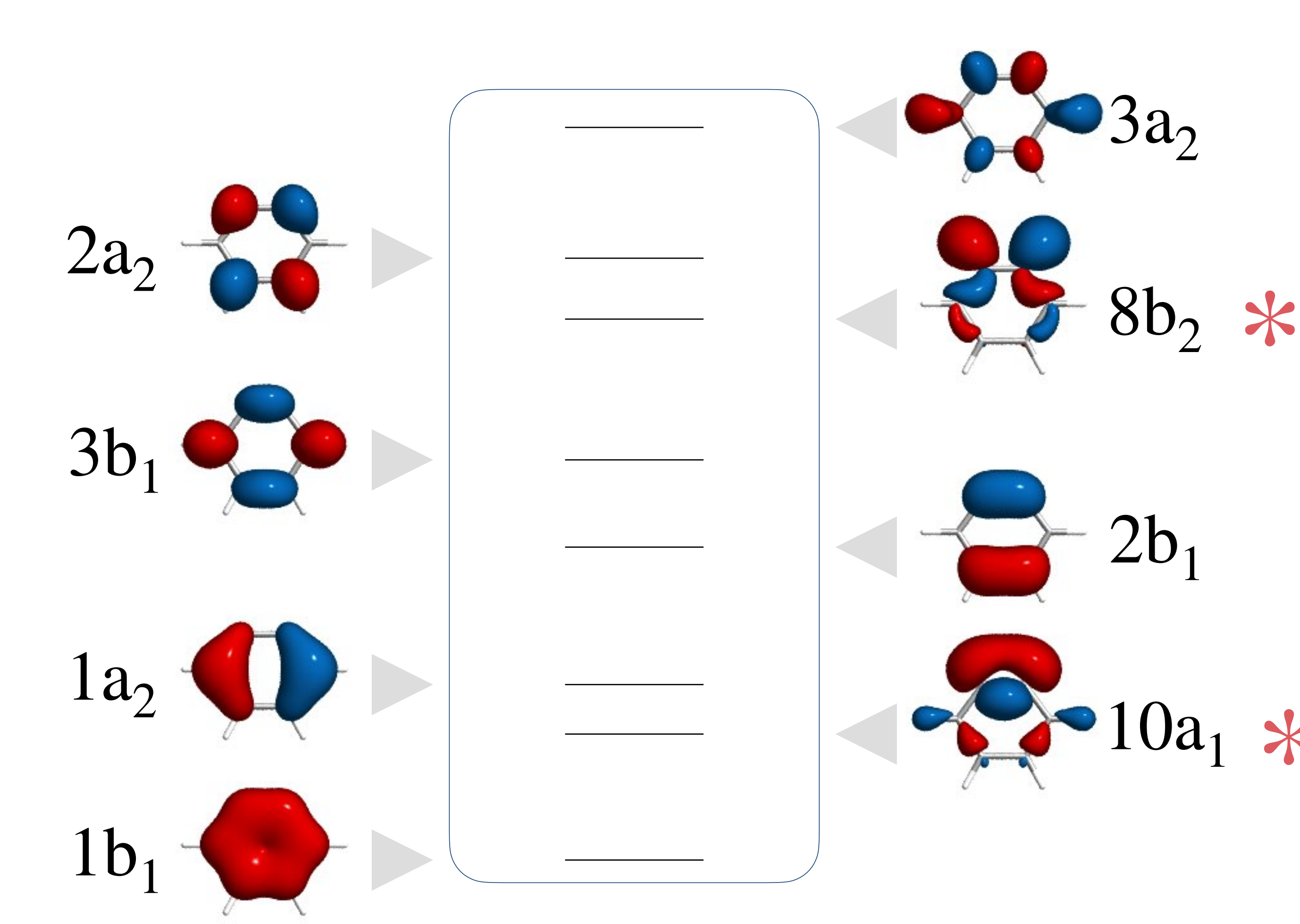
para-benzyne



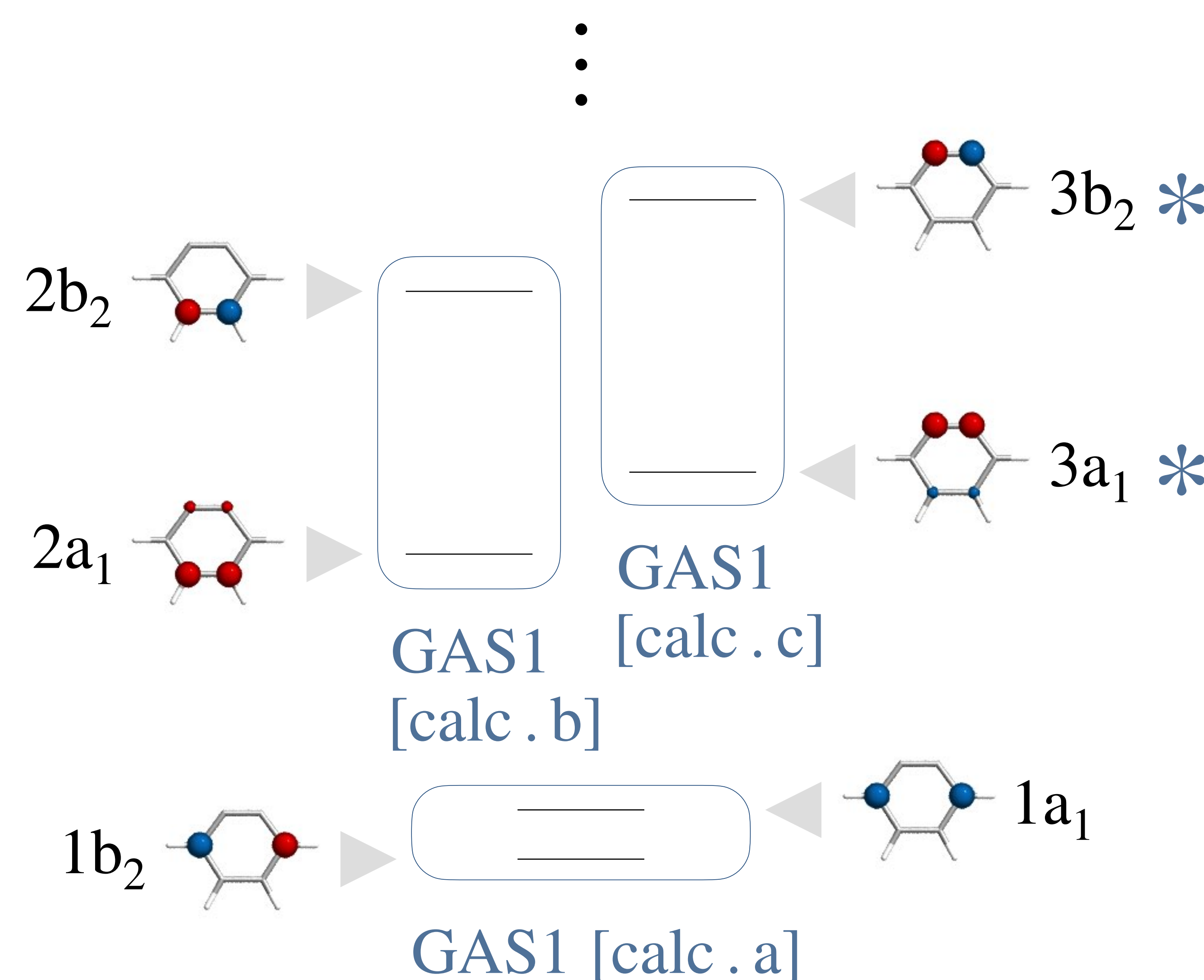
GAS2 [calc . a-d]



meta-benzyne



GAS2 [calc . a-c]



ortho-benzyne

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

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