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Addition/Correction

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Correction to Walsh Diagrams: Molecular Orbital and Structure Computational Chemistry Exercise for Physical Chemistry

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Results for both Hartree−Fock (HF) and MP2 calculations were provided in this activity.[1] As indicated in the SI, MP2 uses perturbation theory to find corrections to the energy (to account for electron correlation). Although corrections to the wave function may be determined using perturbation theory in general, the orbitals MP2 reports are the HF orbitals. As such, there is no additional information contained in the orbitals reported by MP2 compared to the HF orbitals. Those using this activity should therefore work with DFT and either HF or MP2 rather than all three. The authors thank Dr. Paul Jasien for his insight into the MP2 orbital calculation.

REFERENCES

(1) Miller, C. S.; Ellison, M. Walsh Diagrams: Molecular Orbital and Structure Computational Chemistry Exercise for Physical Chemistry. *J. Chem. Educ.* **2015**, *92* (6), 1040−1043.

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