Additional Reading Material

General Information about ORCA software

ORCA is a general-purpose quantum chemistry program package that features virtually all modern electronic structure methods.

ORCA uses standard Gaussian basis functions. Due to its user-friendly style, ORCA is considered to be a helpful tool not only for computational chemists, but also for chemists, physicists and biologists who are interested in developing full information content of their experimental data with the help of calculations. Its main field of application is larger molecules, transition metal complexes, and their spectroscopic properties.

ORCA was developed in the research group of Frank Neese. The free version is available only for academic use at academic institutions.

More information on ORCA is available on these websites.

https://hpc.hku.hk/hpc/software/orca/

https://en.wikipedia.org/wiki/ORCA_(quantum_chemistry_program)

https://www.orcasoftware.de/tutorials_orca/bib.html

To work with ORCA users must be familiar with topics in Computational Chemistry.

Suggested reading:

Essentials of computational chemistry - Christopher J. Cramer.
Introduction to Computational Chemistry – Frank Jensen.

Modern Quantum Chemistry by Szabo and Ostlund.

Computational Chemistry and Molecular Modeling: Principles and Applications by K I Ramachandran and Gopakumar Deepa.

Computational Chemistry: A Practical Guide for Applying Techniques to Real World Problems by David C. Young