Additional Reading Material

General Information about ORCA software

ORCA is a quantum/computational chemistry software for electronic structure calculations. ORCA is developed in the research group of Prof. Frank Neese in Max Planck Institute. Free version of ORCA is available only for academic use at academic institutions. To work with ORCA users must be familiar with topics in computational chemistry.

ORCA uses standard Gaussian functions for basis sets. ORCA is a popular program among chemists, physicists and biologists who are interested in developing the 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 does not have a GUI. It is best used in conjunction with software which have a GUI, such as Avogadro, Jmol, to view and display the result.

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

Suggested reading:

Essentials of computational chemistry - Christopher J. *Cramer*.
Introduction to Computational Chemistry – Frank Jensen.
Modern Quantum Chemistry by Szabo and Ostlund.

1. Computational Chemistry and Molecular Modeling: Principles and Applications by K. I Ramachandran and Gopakumar Deepa.
2. Computational Chemistry: A Practical Guide for Applying Techniques to Real World Problems by David C. Young

.