Improving quantum chemistry workflows with cclib: enabling easier post-processing by universally representing quantum chemistry logfiles

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Over the past decade, cclib has assisted computational chemistry practitioners by handling output file parsing, enabling the post-processing of parsed data, and providing a bridge between external software packages. The field of computational chemistry uses computational tools to describe the structures, mechanisms, and properties of molecules and solids. However, in most cases, software packages do not produce machine-readable output, which results in ever-recreated, error-prone scripts. Additionally, many computational chemistry software packages were created in isolation from one another, leading to variation in output style, data conventions, and calculation capabilities. Cclib is a Python package which aims to address these challenges to improve the data analysis and compatibility between software packages. Cclib parses output from many different quantum chemistry programs into a unified data representation, which allows bridging between various codes such as ASE, Avogadro, Biopython, Horton, Psi4, and PySCF. From this unified data representation one can perform post-processing calculation methods such as population analysis, charge analysis, fragments, and electric multipole moments. This poster highlights how cclib contributes to reducing barriers for data analysis and workflows in computational chemistry, as well as demonstrates the ease of use with examples.