Example for quantum-chemistry-bonn

Christian Selzer & Lukas Wittmann June 5, 2025

1 Introduction

In this document, it is demonstrated how to use abbreviations and colors from quantum-chemistry-bonn.

1.1 Abbreviations

Here are a few examples:

- Calculations were performed with ORCA
- The best program is xTB for SQM and it has no bugs.
- The energy is 5 kcal mol⁻¹. Another energy is 4 kJ mol⁻¹.
- Energies were calculated on the r²SCAN-3c, or just use r²SCAN-3c level of theory. Sadly, no-one wants to use ω Pr²SCAN50-D4.

1.2 Colored Elements

- Here something is written in blue, optionally also via \colb{}.
- For comparison something in normal blue.

2 Conclusion

The package offers simple abbreviations and colors that are maintained centrally in one file.