

quantum-chemistry-bonn Package Documentation

Christian Selzer & Lukas Wittmann

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Abstract

This document describes the `quantum-chemistry-bonn` package (version 0.2, dated 2026/03/12), developed to consolidate common quantum-chemistry program names, colorful branding elements, and frequently used abbreviations into a single, centrally maintained style file. With `quantum-chemistry-bonn`, authors can ensure uniform formatting for program names, method labels, color highlights, and other notations across all QC-related manuscripts.

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1 Introduction

The `quantum-chemistry-bonn` package was created to simplify and standardize the appearance of quantum-chemical program names, method labels, and key notations in \LaTeX documents. Rather than manually inserting font switches, colors, or special macros each time you mention a program (e.g., ORCA, `xTB`) or a quantity (e.g., pK_a , $\Delta_{\text{solv}}G$), `quantum-chemistry-bonn` provides a concise set of commands that automatically apply consistent formatting. Additionally, several custom colors matching the University of Bonn's corporate palette are defined, enabling easy color highlights in presentations, posters, or manuscripts.

Key features:

- **Program Macros:** Uniform fonts (small caps, typewriter) for popular QC codes (`ORCA`, `CENSO`, `DRACO`, `CREST`, `xTB`, `tblite`).
- **Color Palette:** Predefined RGB colors (e.g., `bonnblue`, `bonnred`, `bonnyellow`, `bonngreen`) aligned with University of Bonn branding.
- **Reference Shortcuts:** Quick macros for cross-referencing (`\figref`, `\tabref`, `\eqqref`, `\siref`).
- **Abbreviation Macros:** Convenient commands for *et al.*, *i.e.*, *e.g.*, and physical chemistry quantities (pK_a , $\Delta_{\text{solv}}G$, kcal mol^{-1} , etc.).
- **QC-Method Macro:** Shorthands for several quantum mechanical methods such as `r2SCAN-3c` and `ω B97M-V`.
- **Acronym Definitions:** Over 80 predefined acronyms for common QC terminology (e.g., density functional theory (DFT), basis set superposition error (BSSE), coupled cluster (CC)) via the `acronym` package.
- **Dependencies:** `xcolor`, `siunitx`, `expl3/xparse`, and `acronym`.

2 Installation

2.1 CTAN or Local

The `quantum-chemistry-bonn` package is available via CTAN. Add the following line in your document's preamble:

```
\usepackage{quantum-chemistry-bonn}
```

2.2 Manual (Unpacked) Usage

If you have not installed the package system-wide, simply place `quantum-chemistry-bonn.sty` in the same folder as your `.tex` document. Then, in the preamble:

```
% If quantum-chemistry-bonn.sty is in the same directory:  
\input{quantum-chemistry-bonn.sty}
```

3 Color Definitions

`quantum-chemistry-bonn` defines a palette of RGB colors aligned with the University of Bonn branding, plus a few additional utility colors. All color names can be passed to `\textcolor{<name>}{...}` or used in other color-aware commands.

| Color Name | RGB | Description |
|-----------------------------|-----------------|------------------------------------------------------|
| <code>bonnblue</code> | (007, 078, 159) | “Bonn blue” primary corporate color. |
| <code>bonnred</code> | (185, 039, 039) | “Bonn red” accent color. |
| <code>bonnyellow</code> | (252, 186, 000) | “Bonn yellow” highlight. |
| <code>bonngrey</code> | (144, 144, 133) | Neutral grey tone. |
| <code>bonngray</code> | (144, 144, 133) | Alias for <code>bonngrey</code> (American spelling). |
| <code>bonngreen</code> | (000, 123, 078) | Contrast green for accent. |
| <code>newaccent</code> | (000, 000, 000) | Reserved for future accent. |
| <code>black</code> | (000, 000, 000) | Standard black (redundant with default). |
| <code>highlightgreen</code> | (000, 204, 000) | Bright green for highlighting. |
| <code>white</code> | (255, 255, 255) | Pure white (contrast). |
| <code>StdBody</code> | (233, 233, 233) | Light grey for backgrounds or shading. |

3.1 Usage Examples

```
% Text in Bonn blue:
\textcolor{bonnblue}{This text appears in Bonn blue.}

% Using shortcut macros:
\colb{This is also Bonn blue.}
\colr{This text is Bonn red.}
\colg{This text is Bonn grey.}
\coly{This text is Bonn yellow.}
```

4 Shortcut Color Macros

To simplify inline color usage, quantum-chemistry-bonn defines four “short-cut” macros:

- `\colb{<text>}` ⇒ blue text.
- `\coly{<text>}` ⇒ yellow text.
- `\colr{<text>}` ⇒ red text.
- `\colg{<text>}` ⇒ grey text.

Example:

This sentence has a `\colb{blue phrase}`, a `\colr{red phrase}`, and a `\coly{yellow phrase}`.

5 Reference Shortcut Macros

quantum-chemistry-bonn provides four convenience macros for common cross-reference patterns:

`\figref{<label>}` – Renders “Fig. `\ref{<label>}`”.

Usage:

As shown in `\figref{fig:energy}`, the barrier is small.

`\tabref{<label>}` – Renders “Tab. `\ref{<label>}`”.

Usage:

The full data is listed in `\tabref{tab:results}`.

`\eqqref{<label>}` – Renders “Eq. `\ref{<label>}`”.

Usage:

Substituting into `\eqqref{eq:schroedinger}` gives ...

`\siref{<text>}` – Renders “Supplemental Material, *itext*”.

Usage:

Further details are given in `\siref{Table S1}`.

6 Program Name Macros

Quantum-chemistry program names often involve unconventional capitalization, spacing, or font choices. `quantum-chemistry-bonn` provides dedicated macros to ensure consistent formatting. All program-related commands use `\newcommand*` and select an appropriate font shape:

`\orca` – Renders “ORCA” using the AvantGarde font family.

Usage:

Calculations were performed with `\orca\`.

`\censo` – Renders “CENSO” in the same monospaced style.

Usage:

`\censo\` was employed for ensemble refinements.

`\draco` – Renders “Draco” in small caps.

Usage:

`\draco\` yields improved solvation energies.

`\crest` – Renders “CREST” in small caps.

Usage:

Conformers were generated with `\crest\`.

`\xtb` – Renders “xTB” in a `\texttt` (typewriter) font.

Usage:

For fast SQM screening, we used `\xtb\`.

`\tblite` – Renders “tblite” in a `\texttt` font.

Usage:

Hamiltonian elements were calculated via `\tblite\`.

Note: Each macro adds an implicit, unbreakable space at the end. If you do not want a space (e.g., before punctuation), use `\orca{}` or manual spacing.

7 Miscellaneous Macros

In addition to program names, `quantum-chemistry-bonn` defines several commonly used scientific abbreviations and units:

`\etal` – Renders “*et al.*”.

Usage:

Smith `\etal\` reported similar results.

`\ie` – Renders “*i.e.*”.

Usage:

We used the B3LYP functional (`\ie\` hybrid GGA).

`\eg` – Renders “*e.g.*”.

Usage:

Many packages (`\orca`, `\xtb`) compute dispersion.

`\pka` – Renders “ pK_a ” with a proper subscript “ a ”.

Usage:

The calculated `\pka\` of the acid is 4.8.

`\dgsolv` – Renders “ $\Delta_{\text{solv}}G$ ” (solvation free energy).

Usage:

The `\dgsolv\` was computed with SMD.

`\kcalpmol` – Renders “ kcal mol^{-1} ” using `siunitx`.

Usage:

The reaction barrier is 15.2 `\kcalpmol`.

`\kjpmol` – Renders “ kJ mol^{-1} ” using `siunitx`.

Usage:

The binding energy is 63.6 `\kjpmol`.

`\logunits` – Renders “log units” using `siunitx`.

Usage:

The RMSE amounts to 0.4 `\logunits`.

`\logkow` – Renders “ $\log K_{o/w}$ ” (octanol/water partition coefficient).

Usage:

The `\logkow\` value indicates moderate lipophilicity.

`\logkaw` – Renders “ $\log K_{a/w}$ ” (air/water partition coefficient).

Usage:

The `\logkaw` was estimated from SMD calculations.

`\logkab` – Renders “ $\log K_{\alpha/\beta}$ ” (α/β partition coefficient).

Usage:

The `\logkab` describes the phase partitioning.

`\logpl` – Renders “ $\log P_L$ ” (liquid-phase vapor pressure).

Usage:

The `\logpl` was obtained experimentally.

8 QC-Method Macro

quantum-chemistry-bonn includes dedicated macros for popular quantum mechanical methods:

`\method{<method>}` – Renders `<method>` using a case-insensitive lookup. If the method key is recognized, the properly formatted version is returned; otherwise the raw input is echoed back.

Usage:

Single-point energies were obtained at the `\method{r2scan3c}` level of theory.

Currently declared methods and their accepted aliases:

| Rendered Output | Accepted Keys (any case) |
|---------------------------------------------------------|------------------------------------------|
| <code>r²SCAN-3c</code> | <code>rsc, r2scan3c, r2scan-3c</code> |
| <code>ωB97M-V</code> | <code>wb97mv, wb97m-v</code> |
| <code>ωr²SCAN-D4</code> | <code>wr2scand4, wr2scan-d4</code> |
| <code>ωPr²SCAN50-D4</code> | <code>wpr2scan50d4, wpr2scan50-d4</code> |

Users can register additional methods in their preamble:

- `\DeclareMethod{<key>}{<formatted>}`
- `\DeclareMethods{<key1>,<key2>,...}{<formatted>}`

9 Acronym Definitions

Starting with version 0.2, `quantum-chemistry-bonn` ships with over 80 predefined acronyms for quantum-chemistry terminology, powered by the `acronym` package (loaded with the `[nolist]` option). On first use, `\ac{<key>}` expands to the full form followed by the abbreviation in parentheses; subsequent uses print only the abbreviation.

Key commands (provided by the `acronym` package):

`\ac{<key>}` – Standard use: full form on first occurrence, short form thereafter.

`\acf{<key>}` – Force full form (long + short).

`\acs{<key>}` – Force short form only.

`\acl{<key>}` – Force long form only.

`\acp{<key>}` – Plural version.

`\acresetall` – Reset all acronyms to “first use” state.

Example:

```
The \ac{dft} calculations were done ... % first use
Further \ac{dft} results confirm ... % short form
The \ac{bsse} was corrected via \ac{cp}.
```

Selected predefined acronyms (excerpt):

| Key | Short | Long Form |
|------------|--------------|-------------------------------------------------|
| dft | DFT | density functional theory |
| dftb | DFTB | density functional tight-binding |
| wft | WFT | wave function theory |
| hf | HF | Hartree-Fock |
| cc | CC | coupled cluster |
| mp2 | MP2 | second-order Møller-Plesset perturbation theory |
| dfa | DFA | density functional approximation |
| bsse | BSSE | basis set superposition error |
| bsie | BSIE | basis set incompleteness error |
| scf | SCF | self-consistent field |
| ri | RI | resolution of the identity |
| ecp | ECP | effective core potential |
| nci | NCI | non-covalent interaction |
| rmse | RMSE | root mean square error |
| mae | MAE | mean absolute error |
| m1 | ML | machine learning |
| pes | PES | potential energy surface |
| nmr | NMR | Nuclear Magnetic Resonance |
| x2c | X2C | exact two-component |
| gga | GGA | generalized gradient approximation |

For the complete list of all predefined acronyms, see the source file `quantum-chemistry-bonn.sty`. Users can add custom acronyms in their preamble via:

```
\acronym{<key>}[<short>]{<long>}
```

10 Example Usage

Below is a minimal working example showing how to load the package and use its macros. Copy the following into a file named `example-quantum-chemistry-bonn.tex` and compile with L^AT_EX:

```
\documentclass[a4paper,12pt]{article}

% If installed system-wide:
% \usepackage{quantum-chemistry-bonn}
% Otherwise, place quantum-chemistry-bonn.sty in tex/:
```

```

\input{tex/quantum-chemistry-bonn.sty}

\title{Example for \texttt{quantum-chemistry-bonn}}
\author{Christian Selzer}
\date{\today}

\begin{document}
\maketitle

\section{Introduction}
In this document, we demonstrate how to use
the \texttt{quantum-chemistry-bonn} package.

\subsection{Abbreviations}
Here are a few examples:
\begin{itemize}
\item Calculations were done with \orca\.
\item We used \xtb\ for SQM screening.
\item Smith \etal\ found \rsc\ accurate.
\end{itemize}

\subsection{Colored Elements}
\begin{itemize}
\item Text in \textcolor{bonnblue}{blue},
or via \verb|\colb{}|.
\item Compare: \textcolor{blue}{normal blue}.
\item Highlighted: \coly{Bonn yellow}.
\end{itemize}

\section{Conclusion}
The package offers abbreviations and colors
maintained centrally in one file.

\end{document}

```

After compilation, the PDF will show all macros in action. Adjust paths as needed.

11 License and Credits

`quantum-chemistry-bonn` is distributed under the LaTeX Project Public License (LPPL) as specified by the author. By using this package, you agree to abide by the terms of the license. For full license text, please refer to the LICENSE file that accompanies this package.

Author: Christian Selzer & Lukas Wittmann

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12 Future Directions

Possible enhancements in future releases:

- Add user-configurable options for toggling individual macros or redefining color values.
- Introduce additional program names (e.g., Q-Chem, Gaussian, Psi4) as macros.
- Provide support for colored hyperlinked URLs matching the corporate palette.
- Extend with macros for common basis sets or density functionals.