`quantum-chemistry-bonn` Package Documentation

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Abstract

This document describes the `quantum-chemistry-bonn` package (version 0.1, dated 2025/06/03), 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, δG_solv), `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 (`bonnblue`, `bonnred`, `bonnyellow`, `bonngrey`/`bonngray`, `bonngreen`, etc.) aligned with University of Bonn branding.
- **Abbreviation Macros:** Convenient commands for *et al.*, *i.e.*, *e.g.*, physical chemistry quantities (pK_a, δG_solv, kcal mol^{-1}).
- **QC-Method Macro:** Shorthands for several quantum mechanical methods such as r^{2}SCAN-3c .
- **Minimal Dependencies:** Only `xcolor` and `siunitx` are required.

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 the `quantum-chemistry-bonn.sty` file in the same folder as your `.tex` document. Then, in the preamble, either:

```
% 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
`bonnblue`	(007, 078, 159)	"Bonn blue" primary corporate color.
`bonnred`	(185, 039, 039)	"Bonn red" accent color.
`bonnyellow`	(252, 186, 000)	"Bonn yellow" highlight.
`bonngrey`	(144, 144, 133)	Neutral grey tone.
`bonngray`	(144, 144, 133)	Alias for `bonngrey` (American spelling).
`bonngreen`	(000, 123, 078)	Contrast green for accent.
`newaccent`	(000, 000, 000)	Reserved for future accent.
`black`	(000, 000, 000)	Standard black (redundant with default).
`highlightgreen`	(000, 204, 000)	Bright green for highlighting.
`white`	(255, 255, 255)	Pure white (contrast).
`StdBody`	(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 "shortcut" 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 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" in a monospaced (typewriter) font via `\fontfamily{pag}`.
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:

```
The new module in \draco\ yields improved solvation free 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.

6 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 (e.g., \orca, \xtb) can compute dispersion.
```

`\pka` – Renders "pK_a" with a proper subscript "a".
Usage:

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

`\dgsolv` – Renders "δG_solv" with the delta and subscript "solv".
Usage:

```
The solvation free energy (\dgsolv) was computed using SMD.
```

`\kcalmol` – Renders "kcal·mol^{-1} " with a trailing thin space to separate it from the next word.
Usage:

```
The reaction barrier is 15.2 \kcalmol.
```

7 QC-Method Macro

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

`\method{<method>}` – Renders `<method>` properly e.g. "r^{2}SCAN-3c" with proper superscript formatting for the "2".
Usage:

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

8 Example Usage

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

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

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

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

\begin{document}
\maketitle

\section{Introduction}
In this document, it is demonstrated how to use abbreviations and colors from \t

\subsection{Abbreviations}
Here are a few examples:
\begin{itemize}
  \item Calculations were performed with \orca\.
  \item The best program is \xtb\ for SQM and it has \emph{no} bugs.
  \item As shown by Smith \etal, the method \rsc\ is accurate.
\end{itemize}

\subsection{Colored Elements}
\begin{itemize}
    \item Here something is written in \textcolor{bonnblue}{blue}, optionally al
    \item For comparison something in \textcolor{blue}{normal blue}.
    \item Highlighted text in \coly{Bonn yellow}.
\end{itemize}

\section{Conclusion}
The package offers simple abbreviations and colors that are maintained centrally

\end{document}
```

After compilation, the PDF will show all macros in action. Adjust paths as needed (e.g., `src/quantum-chemistry-bonn.sty` vs. `quantum-chemistry-bonn.sty`).

9 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.

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10 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.