The `orbitals` package

Atomic subshell / orbital-box diagrams with automatic electron filling

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Abstract

`orbitals` draws the familiar "box-and-arrow" notation for atomic subshells (s, p, d, f). You supply only the principal quantum number, the subshell type and the number of electrons; the package places the electrons automatically following *Hund's rule* (maximum multiplicity) and the *Pauli principle*. It can draw a single subshell, a sequence of subshells, a complete valence configuration with a noble-gas core, or an empty transition-series template. Every diagram can be scaled and dropped inline inside running text.

Contents

1 Requirements and installation

The package requires a TeX system no older than 2020 and the TikZ/pgf bundle. It works with pdfLaTeX, XeLaTeX and LuaLaTeX. TikZ, xcolor and graphicx are loaded automatically; mhchem is loaded only if present (used by the optional `\chem` helper).

Manual installation. Place `orbitals.sty` either in the same folder as your document or in your local `texmf` tree, e.g.

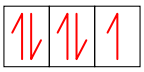
```
TEXMFHOME/tex/latex/orbitals/orbitals.sty
```

then run `texhash` (for a TDS tree). Load it with:

```
\usepackage{orbitals}
```

2 Quick start

```
\suborbital{4}{p}{5}
```

Result: $4p^5$ 

The three mandatory arguments are always *principal quantum number*, *subshell letter* and *number of electrons*. The number of boxes is chosen from the letter: $s \to 1$, $p \to 3$, $d \to 5$, $f \to 7$.

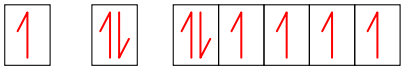
3 Command reference

3.1 `\suborbital` – a single subshell

```
\suborbital[<scale>]{<n>}{<type>}{<electrons>}
```

The optional `<scale>` defaults to the global scale (Section 4.1).

```
\suborbital{4}{s}{1}   \suborbital{4}{s}{2}   \suborbital{3}{d}{6}
```

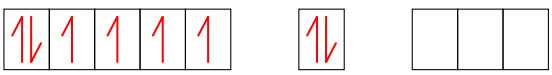
Result: $4s^1$ $4s^2$ $3d^6$ 

3.2 `\electronconfig` – a sequence

```
\electronconfig[<scale>]{<n><type><electrons>, ...}
```

Each item uses the compact form `4p5` (one digit for n, one letter for the type, the rest for the electron count, so `3d10` is fine).

```
\electronconfig{3d6,4s2,4p0}
```

Result: $3d^6$ $4s^2$ $4p^0$ 

3.3 `\atomconfig` – configuration with a core

```
\atomconfig[<core>][<gap-cm>][<scale>]{<list>}
```

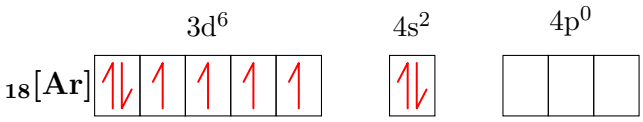
- `<core>`: text of the noble-gas core (default: empty).

- `<gap-cm>`: horizontal space (in cm) reserved before the first box (default `1`).
- `<scale>`: scale factor (default: the global scale).

Important: if the core text itself contains a closing bracket `]` (as in `[Ar]`), wrap the whole core in braces so LaTeX does not end the optional argument early:

```
\atomconfig[{\textsubscript{18}[Ar]}][1.2]{3d6,4s2,4p0}
```

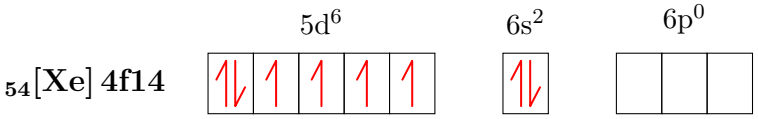
Result:



Wide cores simply need a larger gap:

```
\atomconfig[{\textsubscript{54}[Xe]\,4f14}][2.7]{5d6,6s2,6p0}
```

Result:



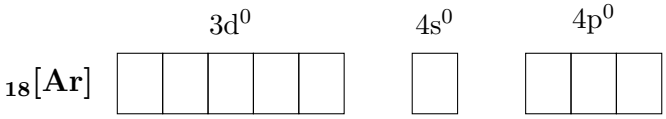
3.4 `\transitionseries` – empty templates

```
\transitionseries[<scale>]{<1|2|3>}
```

Draws an empty $d/s/p$ frame for the first (1), second (2) or third (3) transition series, with the appropriate noble-gas core.

```
\transitionseries{1}
```

Result:



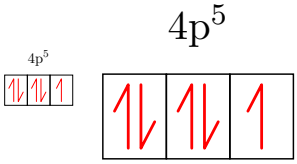
4 Customisation

4.1 Scaling

Two mechanisms are available. A *per-call* optional argument:

```
\suborbital[0.5]{4}{p}{5}   \suborbital[1.4]{4}{p}{5}
```

Result:



and a *global* setting applied to all subsequent diagrams:

```
\setOrbitalScale{0.7}   % everything afterwards is 70%
\setOrbitalScale{1}     % back to normal
```

4.2 Inline placement and vertical alignment

Diagrams are vertically centred on the text line by default, so they sit naturally at the beginning, middle or end of a sentence. Switch the alignment with:

```
\setOrbitalAlign{center}  % centred on the line (default)
\setOrbitalAlign{bottom}  % sitting on the baseline
```

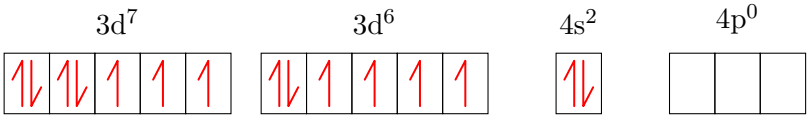
For example, the Fe^{3+} ion has a  half-filled configuration.

Here it sits on the line For example, the Fe^{3+} ion has a  like this.

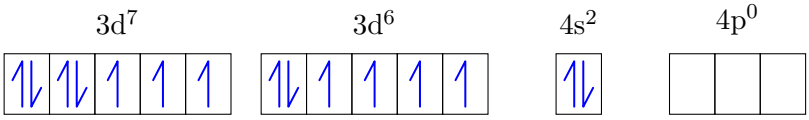
4.3 Colours, box size and spacing

```
\setElectronColor{blue}   % arrow colour (default red)
\setOrbitalBox{0.8}{1.0}  % {box width}{box height} in cm
\setOrbitalGap{0.9}       % gap between subshells in cm
```

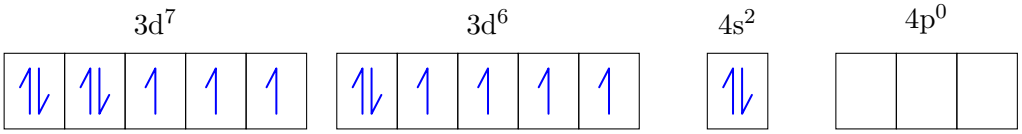
Default:



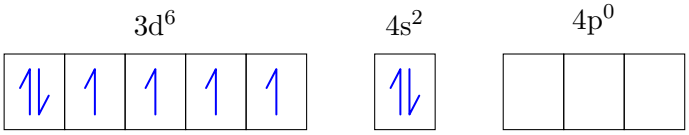
arrow colour `\setElectronColor{blue}`



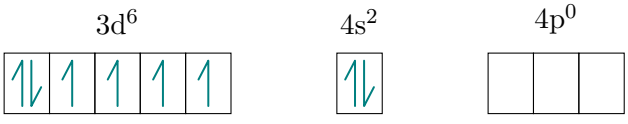
box size `\setOrbitalBox{0.8}{1.0}`



gap `\setOrbitalGap{0.9}`



all three together:



4.4 Arrow shape

Electrons are drawn as half-arrows (TikZ `pics` `halfarrowup` / `halfarrowdown`). Adjust them with:

```
\setElectronArrow{<stem length>}{<line width>}  % e.g. {0.5}{1.2pt}
```

4.5 The `\chem` helper

If mhchem is available, `\chem{Fe^3+}` typesets a formula via `\ce`.

5 How electrons are placed

For a subshell with k boxes and N electrons the package computes the number of doubly occupied boxes as $\max(0, N - k)$ and fills the remaining electrons as single "spin-up" arrows. This reproduces the high-spin (free-atom) ground state expected from Hund's rule and the Pauli principle. Low-spin (complex) fillings are not produced automatically.

6 Command summary

`\suborbital[s]{n}{t}{e}`	one subshell
`\electronconfig[s]{list}`	a row of subshells
`\atomconfig[core][gap][s]{list}`	configuration with a core
`\transitionseries[s]{1|2|3}`	empty transition template
`\setOrbitalScale{f}`	global scale
`\setOrbitalAlign{center|bottom}`	inline alignment
`\setElectronColor{c}`	arrow colour
`\setOrbitalBox{w}{h}`	box size (cm)
`\setOrbitalGap{g}`	subshell gap (cm)
`\setElectronArrow{stem}{lw}`	arrow geometry

7 License and version history

This package is distributed under the LaTeX Project Public License (LPPL) version 1.3c .

v1.0 (2026/05/24): first public release.