

How to write magnetic point groups symbols using 'RI' notation in L^AT_EX?

supplement to article:

"Magnetic, electric and toroidal polarisation modes describing the physical properties of crystals. NdFeO₃ case"

Piotr Fabrykiewicz*, Radosław Przeniosło and Izabela Sosnowska

*Correspondence e-mail: Piotr.Fabrykiewicz@fuw.edu.pl

Acta Cryst. **A79** (2023), <https://doi.org/10.1107/S2053273322009858>

In L^AT_EX file preamble include following lines (can be easily copied from .tex source of this .pdf):

```
\usepackage{xcolor}
\newcommand*\blue[1]{\textcolor{blue}{\ensuremath{\bar{\#1}}}}
\newcommand*\red[1]{\textcolor{red}{\ensuremath{\#1'}}}
\newcommand*\green[1]{\textcolor{green}{\ensuremath{\bar{\#1}'}}}
\usepackage{amsmath}
\newcommand*\bfrac[2]{\genfrac{}{}{0pt}{}{\#1}{\#2}}
\newcommand*\notblue[1]{\ensuremath{\bfrac{\textcolor{red}{\#1'}}{\textcolor{green}{\bar{\#1}'}}}}
\newcommand*\notred[1]{\ensuremath{\bfrac{\textcolor{blue}{\bar{\#1}}}{\textcolor{white}{}{\textcolor{green}{\bar{\#1}'}}}}}
\newcommand*\notgreen[1]{\ensuremath{\bfrac{\textcolor{blue}{\bar{\#1}}}{\textcolor{white}{}{\textcolor{red}{\#1}'}}}}
```

This gives you access to following six commands:

$\backslash\text{blue}\{N\}$, $\backslash\text{red}\{N\}$, $\backslash\text{green}\{N\}$ with $N \in \{1, 2, 3, 4, 6\}$
 $\backslash\text{notblue}\{N\}$, $\backslash\text{notred}\{N\}$, $\backslash\text{notgreen}\{N\}$ with $N \in \{2, 4, 6\}$

Upper commands action is presented below (for $N = 2$):

Command: $\backslash\text{blue}\{2\}$ $\backslash\text{red}\{2\}$ $\backslash\text{green}\{2\}$ $\backslash\text{notblue}\{2\}$ $\backslash\text{notred}\{2\}$ $\backslash\text{notgreen}\{2\}$

Output: $\bar{2}$ $2'$ $\bar{2}'$ $\frac{2'}{\bar{2}'}$ $\frac{\bar{2}}{2'}$ $\frac{\bar{2}}{2'}$

This allow us to easily build any magnetic point group symbol in 'RI' notation e.g.

$422 \rightarrow 422$ $\backslash\text{green}\{4\}\backslash\text{blue}\{2\}\backslash\text{red}\{2\} \rightarrow \bar{4}'\bar{2}2'$ $4\backslash\text{blue}\{2\}\backslash\text{blue}\{2\} \rightarrow 4\bar{2}\bar{2}$
 $422\backslash\text{blue}\{1\}\backslash\text{red}\{1\}\backslash\text{green}\{1\} \rightarrow 422\bar{1}'\bar{1}'$ $422\backslash\text{green}\{1\} \rightarrow 422\bar{1}'$ $\backslash\text{notblue}\{4\}2\backslash\text{notblue}\{2\}\backslash\text{blue}\{1\} \rightarrow \frac{4'}{4}2\frac{2'}{2'}\bar{1}$

Commands works both inside and outside T_EX math mode $\$. . \$$ see following sentences.

Proposed 'RI' notation based on assumption to not distinguish or prioritize any of generalized inversions: $\bar{1}$, $1'$ or $\bar{1}'$.

According to our paper $\bar{6}2'\bar{2}'$, $6'2\bar{2}'$ and $\bar{6}'\bar{2}2'$ groups have the same full-B&W type.

(Please note that .tex source file of this .pdf is also available to download.)