[XeLaTeX-Tips 100106a]

How to Determine the Size of a Structural Formula

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Question:

When two or more structural formulas drawn by XeLaTeX are placed in an equation-like environment without any adjustments, they are badly aligned both vertically and horizontally. How can we correct this type of irregular alignment?

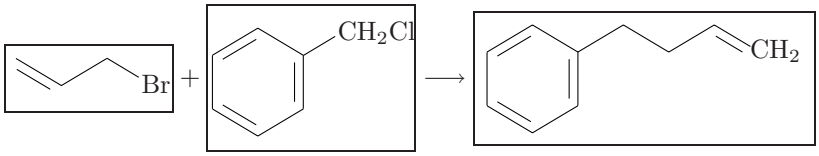
Answer:

Use the XyMcompd environment supported by the chemist or chmst-ps package and determine the sizes of structural formulas to be aligned.

In order to evaluate the domain occupied by each XyMcompd environment, we can conveniently use `\fbox` command. Therby, the first argument (domain values x,y) and the second arument (shift values x,y) of the XyMcompd environment should be determined by trial and error. Because the domain is visualized by the `\fbox` command, our labor of evaluation would be reduced to a greater extent. After several trials of adjusting domain values and shift values, we can obtain the following code:

```
\[
\fbox{%
\begin{XyMcompd}(450,150)(100,150){}{}
\trimethylenei[A]{}{3W==Br}
\end{XyMcompd}%
}
+
\fbox{%
\begin{XyMcompd}(600,450)(300,250){}{}
\bzdrv{2==CH$_{2}$Cl}
\end{XyMcompd}%
}
\longrightarrow
\fbox{%
\begin{XyMcompd}(1100,400)(-100,-100){}{}
\pentamethylene[d]{%
5==CH$_2$;1s==\bzdrv{2==(yl)}}{}
\end{XyMcompd}%
}
\]
```

This code prints out the following equation with frames drawn by the `\fbox` dommand.



Then, the `\fbox` command is deleted or commented out by adding a % symbol (or nullified by introducing `\relax` as follows) so as to give an equation to be desired:

```
\begingroup
\let\fbox=\relax%nullified
\[
\begin{XyMcompd}(450,150)(100,150){}{}
\trimethylenei[A]{}{3W==Br}
\end{XyMcompd}%
\qquad + \qquad
%\fbox %commented out
{%
\begin{XyMcompd}(600,450)(300,250){}{}
\bzdrv{2==CH$_{2}$Cl}
\end{XyMcompd}%
}
\longrightarrow \qquad
\fbox{%nullified by introducing \relax (see above)
\begin{XyMcompd}(1100,400)(-100,-100){}{}
\pentamethylene[d]{%
5==CH$_2$;1s==\bzdrv{2==(yl)}}{}
\end{XyMcompd}%
}
\]
\endgroup
```