[XƎMTEX-Tips 100107a]
Setting Locant Numbers on Atoms

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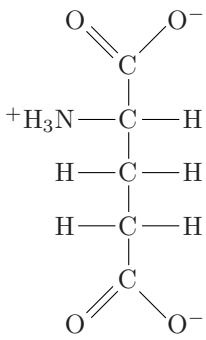
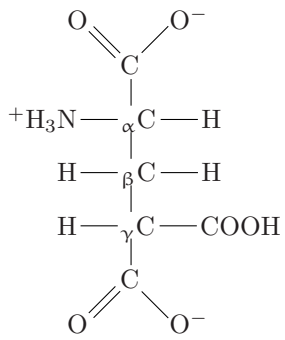
Question:

[Setting locant numbers in XƎMTEX (from tobiwan in AphfelWiki 2009/07/02)] I want to set locant numbers on a xymtex formula. I got as far as the following, but I'd like to have the subscripts more left and not affecting the Carbon-Atoms to shift right. Any suggestions?

```
\begin{center}
\tetrahedral{0==C;1==\utrigonal{0==C;1==(yl);3D==O;2==O$^-$};%
2==$^+$H$_3$N;3==\tetrahedral{%
0==C;1==(yl);2==H;4==H;3==\tetrahedral{0==C;1==(yl);2==H;4==H;
3==\dtrigonal{0==C;1==(yl);2==O$^-$;3D==O}}};4==H}
\hspace{5cm}
\tetrahedral{0==$_{\upalpha}$\vspace{-10pt}C;%
1==\utrigonal{0==C;1==(yl);3D==O;2==O$^-$};
2==$^+$H$_3$N;3==\tetrahedral{%
0==$_{\upbeta}$\vspace{-2pt}C;1==(yl);2==H;4==H;3==%
\tetrahedral{0==$_{\upgamma}$\vspace{-2pt}C;1==(yl);
2==H;4==COOH;3==\dtrigonal{0==C;1==(yl);2==O$^-$;3D==O}}};4==H}
\end{center}
```





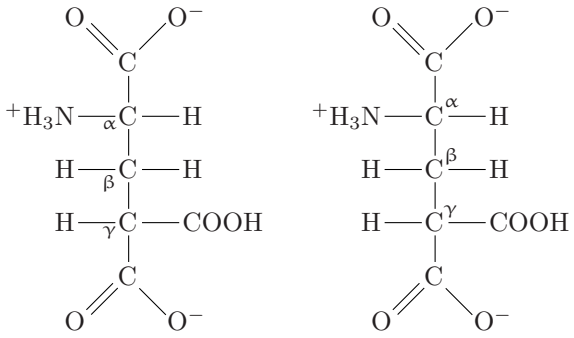
Answer:

[Straightforward Method]

Use the `\llap` or `\rlap` command as follows:

```
%in the preamble:
%\usepackage{xymtexps}
%\usepackage{chmst-ps}
%\verbswitchfalse
%\usepackage{upgreek}
```

```
%
\begin{center}
\begin{XyMcompd}(800,1200)(-100,-500){}{}
\tetrahedral{0==\llap{$_{\upalpha}$}C;1==\utrigonal{0==C;1==(yl);3D==O;2==O$^-$};
2==$^+$H$_3$N;3==\tetrahedral{%
0==\llap{\raisebox{-2pt}{$_{\upbeta}$}}C;1==(yl);2==H;4==H;3==%
\tetrahedral{0==\llap{$_{\upgamma}$}C;1==(yl);
2==H;4==COOH;3==\dtrigonal{0==C;1==(yl);2==O$^-$;3D==O}};4==H}
\end{XyMcompd}
\qquad
\begin{XyMcompd}(800,1200)(-100,-500){}{}
\tetrahedral{0==C\rlap{\raisebox{3pt}{$^{\upalpha}$}};%
1==\utrigonal{0==C;1==(yl);3D==O;2==O$^-$};
2==$^+$H$_3$N;3==\tetrahedral{%
0==C\rlap{\raisebox{3pt}{$^{\upbeta}$}};1==(yl);2==H;4==H;3==%
\tetrahedral{0==C\rlap{\raisebox{3pt}{$^{\upgamma}$}};1==(yl);
2==H;4==COOH;3==\dtrigonal{0==C;1==(yl);2==O$^-$;3D==O}};4==H}
\end{XyMcompd}
\end{center}
```



[Independent Setting of Locant Numbers]

When a locant number is considered to be a substituent or central atom, it can be written in the subslist of each command as if it is an independent node. For this purpose, we should define the following command `\lcntNo` as a hypothetical substituent:

```
\def\lcntNo(#1,#2)#3{\put(#1,#2){\hbox to0pt{\hss\scriptsize #3\hss}}}
```

The first two arguments `(#1,#2)` specify shift values along the x- and y-coordinates. The values `(#1,#2)` are determined by `\unitlength` (=0.1pt) as a unit. Note that the locant number specified by the argument (0,0) is placed just at the original (bottom-left) position of each atom.

Then, the locant `0==\lcntNo(-30,-20){$\upalpha$}` is written in addition ot the atom `0==C`, as shown in the following code:

```
\begin{center}
\begin{XyMcompd}(800,1200)(-100,-500){}{}
\tetrahedral{0==C;0==\lcntNo(-30,-20){$\upalpha$};%
1==\utrigonal{0==C;1==(yl);3D==O;2==O$^-$};
2==$^+$H$_3$N;3==\tetrahedral{%
0==C;0==\lcntNo(-30,-30){$\upbeta$};
1==(yl);2==H;4==H;3==%
\tetrahedral{
0==C;0==\lcntNo(-30,-20){$\upgamma$};1==(yl);%
2==H;4==COOH;3==\dtrigonal{0==C;1==(yl);2==O$^-$;3D==O}};4==H}
\end{XyMcompd}
\qquad
\begin{XyMcompd}(800,1200)(-100,-500){}{}
```

```
\tetrahedral{0==C;0==\lcntNo(100,70){$\upalpha$};%
1==\utrigonal{0==C;1==(yl);3D==O;2==O$^-$};
2==$^+$H$_3$N;3==\tetrahedral{%
0==C;0==\lcntNo(100,70){$\upbeta$};
1==(yl);2==H;4==H;3==%
\tetrahedral{
0==C;0==\lcntNo(100,70){$\upgamma$};1==(yl);%
2==H;4==COOH;3==\dtrigonal{0==C;1==(yl);2==O$^-$;3D==O}}};4==H}
\end{XyMcompd}
\end{center}
```