[XƎMTEX-Tips 100803b]

Cross-Linkage Between Non-Adjacent Positions of a Cyclic Structure

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Question:

I want to draw a bond linking two non-adjacent positions of a cyclic structure. How should I do?

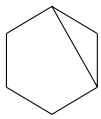
Answer:

Because line slopes of the picture environment of LaTeX are limited to be ratios of two integers between 1 and 6, there are several cases in which two non-adjacent positions cannot be linked properly by means of the technique described in the preceding on-line document (Applications of 100803a.pdf). In order to avoid this shortage of the LaTeX picture environment, we use the `\psline` command defined in the PSTricks package under the PostScript-compatible mode of XƎMTEX (by using `\usepackage{xymtexps}`).

For example, the linkage between 1 and 3 in a six-membered ring drawn by the `\sixheterov` is realized as follows. Thus the code:

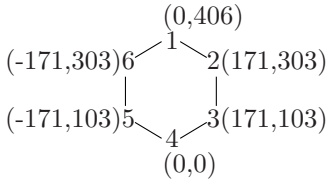
```
\sixheterov{%
1s==\psline[unit=0.1pt,linewidth=0.4pt](0,0)(171,-303)%
}{}
```

produces the following structures:



where the `\psline` command is placed in the atom list of the `\sixheterov` as if it is regarded as a spiro unit. The designation `1s==` means that the line due to `\psline` is started directly at position 1 where the suffix `s` means "saturated skeleton".

It should be noted that the positions of a six-membered ring drawn by the `\sixheterov` is characterized by the following coordinates under `\unitlength=0.1pt` (the unit length of XƎMTEX):



when the 4-position (the bottom position) is selected to be an original point, as shown by the coordinate (0,0).

By referring to these coordinates, the positions 3 and 5 in a six-membered ring drawn by the `\sixheterov` can be linked by the following codes:

```
\sixheterov{%
5s==\psline[unit=0.1pt,linewidth=0.4pt]%
(0,0)(342,0)}{}
%
\sixheterov{%
3s==\psline[unit=0.1pt,linewidth=0.4pt]%
(0,0)(-342,0)}{}
```

which produce the following structures:

When a command for drawing a skeleton structure has no atom list (e.g., `\cyclohexanev`), the `\psline` command is placed in its bond list. For example, the code:

```
\cyclohexanev[%
{a\psline[unit=0.1pt,linewidth=0.4pt](0,0)(171,-303)}%
]{}
%
\cyclohexanev[%
{b\psline[unit=0.1pt,linewidth=0.4pt](0,0)(-171,-303)}%
]{}
%
\cyclohexanev[%
{c\psline[unit=0.1pt,linewidth=0.4pt](0,0)(-342,0)}%
]{}
%
\cyclohexanev[%
{d\psline[unit=0.1pt,linewidth=0.4pt](0,0)(-171,303)}%
]{}
%
\cyclohexanev[%
{e\psline[unit=0.1pt,linewidth=0.4pt](0,0)(171,303)}%
]{}
%
\cyclohexanev[%
{f\psline[unit=0.1pt,linewidth=0.4pt](0,0)(342,0)}%
]{}
```

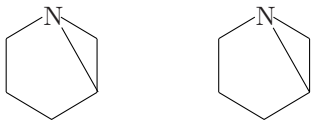
produces the following structures:

Applications

When the terminal position of a cross-linkage contains a hetero atom, the following technique is available. The codes:

```
\sixheterov{%
1==N;%
3s==\psline[unit=0.1pt,linewidth=0.4pt](0,0)(-137,243)}{}
%
\sixheterov[%
{a\psline[unit=0.1pt,linewidth=0.4pt](34,-61)(171,-303)}%
]{1==N}{}
```

produce the following structures:



The coordinates `(0,0)(-137,243)` in the first code designate almost the same slope as `(0,0)(-171,303)`. The coordinates `(34,-61)(171,-303)` in the second code mean that the starting point `(0,0)` of the cross linkage is shifted to `(34,-61)` so as to designate almost the same slope as `(0,0)(171,-303)`.

Chapter 2 (page 19) of the on-line document of XyMTEX version 4.04 (xymtx404.pdf) has shown the structural formula of 3α,5-cyclo-5α-cholestan-6β-ol by writing the code:

```
\steroidChain[%%%%{b\null}%dummy
{b{\psline[unit=0.1pt,linewidth=2pt,%
linestyle=dashed,dash=1pt 1.5pt]%
(6,0)(336,0)}}]
{6B==OH;{10}B==\null;{13}B==\null;%
{17}GA==H;{20}A==\null}
```

where the cross-linkage bond between the positions 3 and 5 is drawn as a dashed line. The resulting structural formula is as follows: