[XƎMTEX-Tips 130204b]
Coordinate Bonds with XƎMTEX

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Question:

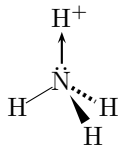
How can I draw coordinate bonds by using XƎMTEX?

Answer:

The lone pair on the nitrogen of an ammonia molecule can form a coordinate bond between the nitrogen and a proton. According to the PostScript mode of XƎMTEX, such a coordinate bond can be drawn after the `\upcoord` command is defined as follows:

```
\documentclass{article}
\usepackage{xymtexps}
\begin{document}
\def\upcoord#1{\psline[unit=0.1pt]{->}(40,100)(40,220)\put(0,240){#1}}
\DtetrahedralS{0==\lonepairA[1]{N};0==\upcoord{H$^+$};2==H;3A==H;4B==H}
\end{document}
```

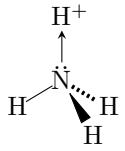
After the LATEX processing, the dvips processing produces a .ps file, which depicts the following structural formula:



On the other hand, the PDF mode of XƎMTEX enables us to draw such a coordinate bond in an alternative way, where another definition of the `\upcoord` command is used as follows:

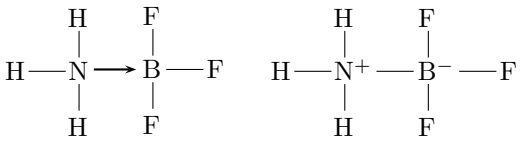
```
\documentclass{article}
\usepackage{xymtexpdf}
\begin{document}
\def\upcoord#1{\tikznodimension{%
\draw[-stealth](40\unitlength,100\unitlength)--%
(40\unitlength,220\unitlength);}\put(0,240){#1}}
\DtetrahedralS{0==\lonepairA[1]{N};0==\upcoord{H$^+$};2==H;3A==H;4B==H}
\end{document}
```

After the LATEX processing, the dvipdfmx processing produces a .pdf file, which depicts the following structural formula:



The lone pair on the nitrogen of an ammonia molecule can form a coordinate bond to overcome the electron deficiency of boron trifluoride. The coordinate bond is represented as follows according to the PostScript-compatible mode of XƎMTEX.

```
\def\rightcoord#1{\psline[unit=0.1pt]{->}(60,40)(220,40)\put(230,40){#1}}
\tetrahedral{0==N;0==\rightcoord{\tetrahedral{0==B;2==(yl);1==F;3==F;4==F}};1==H;2==H;3==H}
\qquad\qquad
\tetrahedral{0==N$^+$;4==\tetrahedral{0==B$^-$;2==(yl);1==F;3==F;4==F};1==H;2==H;3==H}
```



Strictly speaking, the central bond of the N^+—B^- in the second formula is unnecessary, because N^+ B^- or N—B is sufficient to express the bonding. Note that H—Cl or H^+ Cl^- is sufficient, while H^+—Cl^- shows the duplication of bonding.

The S=O bond of dimethyl sulfoxide is drawn variously. The middle formula is drawn by using a newly-defined command `\upcoordd` (the PostScript-compatible mode).

```
\def\upcoordd#1{%
\psline[unit=0.1pt]{->}(0,100)(0,220)\put(-20,240){#1}%
\psline[unit=0.1pt]{-}(40,100)(40,220)}
\Dtrigonal{0==S;1D==O;2==CH$_{3}$;3==H$_{3}$C} \qquad
\Dtrigonal{0==\lonepairA[3]{S};0==\upcoordd{O};2==CH$_{3}$;3==H$_{3}$C} \qquad
\Dtrigonal{0==\lonepairA[3]{S\rlap{$^+$}};1==O$^-$;2==CH$_{3}$;3==H$_{3}$C}
```