[X̃MTEX-Tips 100803a]

Endocyclic Triple Bonds for Drawing Benzyne and Related Structures

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Question:

I want to draw a structure of benzyne, which contains an endocyclic triple bond. However, the options of `\sixheterov` etc. only allow double bonds, because endocyclic triple bonds do not make sense in a normal ring structure. How should I do?

Answer:

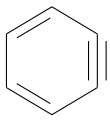
A Rather Dirty Technique

If we rely on existing facilities of X̃MTEX, a rather dirty technique can be applied to this problem, where a fused ring is used with an endocyclic bond and no skeletal bonds. For example,

A code:

```
\sixheterov[bdf{b\sixfusev[e]{}{}{E}[abcdf]}]{}{}
```

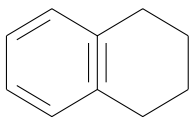
produces the following structure:



Note that the omition of the option [abcdf] from the end of `\sixfusev` command, i.e.,

```
\sixheterov[bdf{b\sixfusev[e]{}{}{E}}]{}{}
```

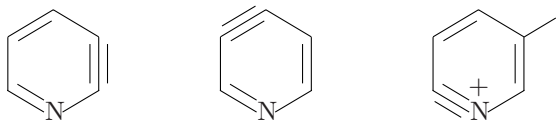
produces a hypothetical fused (chemically impossible) structure without deleting skeletal bonds:



The structures of pyridynes can be drawn by means of this technique. Thus, the codes:

```
\sixheterov[bdf{b\sixfusev[e]{}{}{E}[abcdf]}]{4==N}{}
\sixheterov[bdf{f\sixfusev[c]{}{}{C}[abdef]}]{4==N}{}
\sixheterov[bdf{d\sixfusev[a]{2==}{}{A}[bcdef]}{4+}]{4==N}{2==}
```

produce the following structures:



More Systematic Techniques

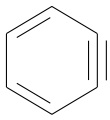
A bond of the slope `(#3,#4)` and of length `#5`, where its terminal is located at the position separated by `(#1,#2)` from a given starting position, can be added by using a newly-defined command:

```
\makeatletter
\def\addbond(#1,#2)(#3,#4)#5{\Put@Line(#1,#2)(#3,#4){#5}}
\makeatother
```

For example, an additional endocyclic bond of benzyne can be drawn by writing the following code:

```
\sixheterov[bdf]{2s==\addbond(30,-25)(0,-1){150}}{}
```

which produces the structure of benzyne as follows:

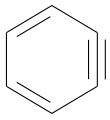


It should be noted that the additional bond is drawn as an endocyclic atom, which is designated in the atom list (`2s==\addbond...`).

Another code:

```
\sixheterov[bdf{b{\addbond(30,-25)(0,-1){150}}}]{}{}
```

where the additional bond is designated in the bond list (`{b{\addbond(30,-25)(0,-1){150}}}`), produces an equivalent structure with an endocyclic triple bond:



Applications

Dewar benzenes can be drawn by using the `\addbond` command. The codes:

```
\sixheterov[be{a{\addbond(0,0)(0,-1){406}}}]{}{}
\sixheterov[be]{1s==\addbond(0,0)(0,-1){406}}{} \par
\sixheterov[cf{b{\addbond(0,0)(-5,-3){342}}}]{}{}
\sixheterov[cf]{2s==\addbond(0,0)(-5,-3){342}}{} \par
\sixheterov[ad{c{\addbond(0,0)(-5,3){342}}}]{}{}
\sixheterov[ad]{3s==\addbond(0,0)(-5,3){342}}{}
```

produce the following structures: