[XeTeX-Tips 100108c]

Skeleton Bonds vs. Substituent Bonds in Zigzag Methylenes

Shinsaku Fujita
Shonan Institute of Chemoinformatics and Mathematical Chemistry

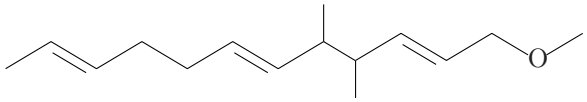
January 7, 2010

Question:

When two long zigzag methylenes are linked by means of the (yl)-function, the linking (yl) bond is shorter than other skeletal bonds. For example, the code:

```
\begin{XyMcompd}(2100,400)(250,50){}{}%
\octamethylene[bf]{}{8W==\hexamethylene[b]{5==O}{1==(yl);1==\null};8==\null}
\end{XyMcompd}
```

generates the following structural formula:



By close inspection of the structure the (yl) bond (between the two methyl side chains) is obviously shorter than the other bonds. How can we elongate the bond into the same length as the other bonds?

Answer:

The (yl) bond at issue is regarded as a bond for linking a substituent, while the other bonds are skeletal bonds. Because such bonds for substitution are decided to be shorter than such skeletal bonds.

To elongate the (yl) bond, the relevant (inner) `\heptamethylenei` (not `\hexamethylene`) is regarded as a spiro unit and written in the atomlist of the outer `\octamethylene`. The resulting code:

```
\begin{XyMcompd}(2100,400)(250,50){}{}%
\octamethylene[bf]{8s==\heptamethylenei[C]{6==O}{1==(yl);2==\null}}{8==\null}
\end{XyMcompd}
```

generates the following structural formula: