Chemical Structures

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Visualizing Chemical Structures

Chemists and students studying Chemistry typically need do draw visual representations of chemical structures. There are several expensive software packages to do this. Examples are ACD Chemsketch which has a free version for personal/academic use. It runs on `Windows 64 bit` computers. ACD Labs notes that it will run on MacOS in a Windows Virtual Machine.

There is also a package called Chem Doodle that runs on Windows, MacOS, and Linux. It sounds great, right? There is a problem: The license costs $15/month or $150/year ot $750/life. Ouch!

Here is the good news: There is an online Open Source Package called MolView. There is a manual (PDF) available here. There is a helpful video by Roger Nixon on YouTube.

One advantage of Molview is that one can find input data for many organic molecules on Pubchem. This link was set to find information on `toluene`. Note that Pubchmem lists an `InChIKey` for toluene: `YXFVVABEGXRONW-UHFFFAOYSA-N`. If one types that key into the Molview `search box` at the top, Molview will draw the structure. That is really helpful.

We can also toggle certain features (like bonds and H) in the display

Export Data

Note what you can export from the `tools` menu:

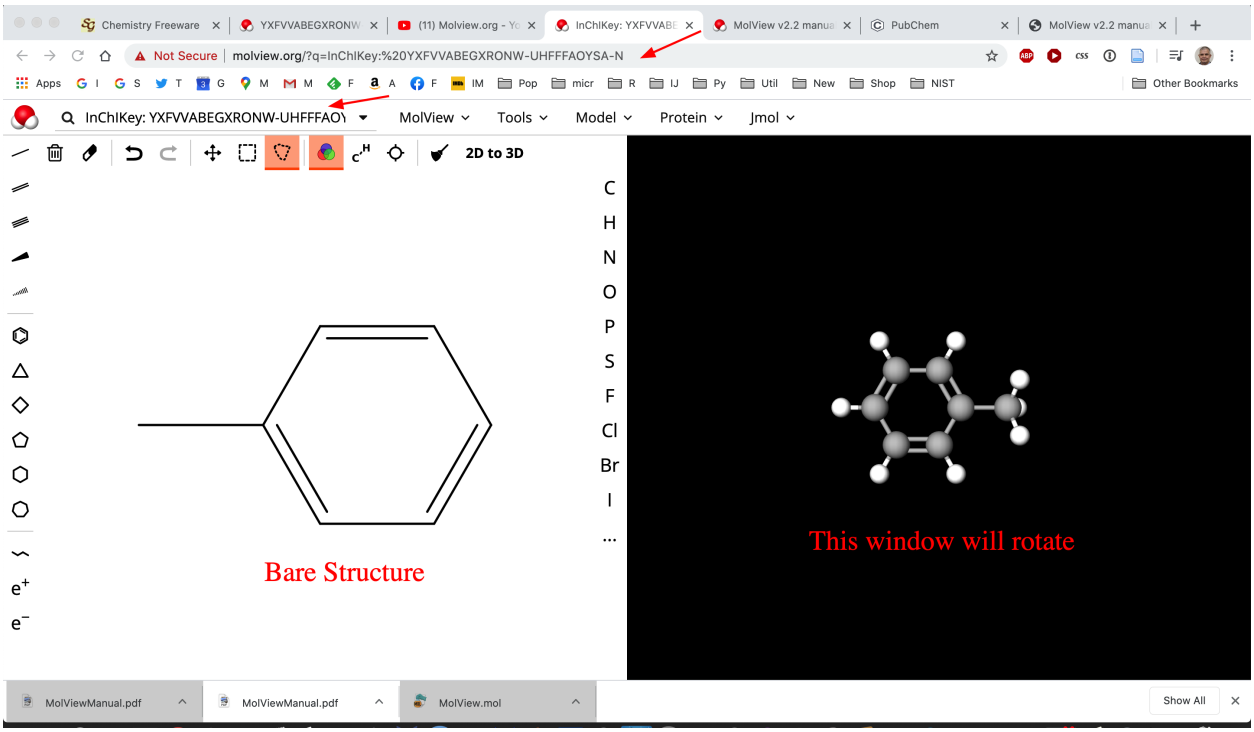
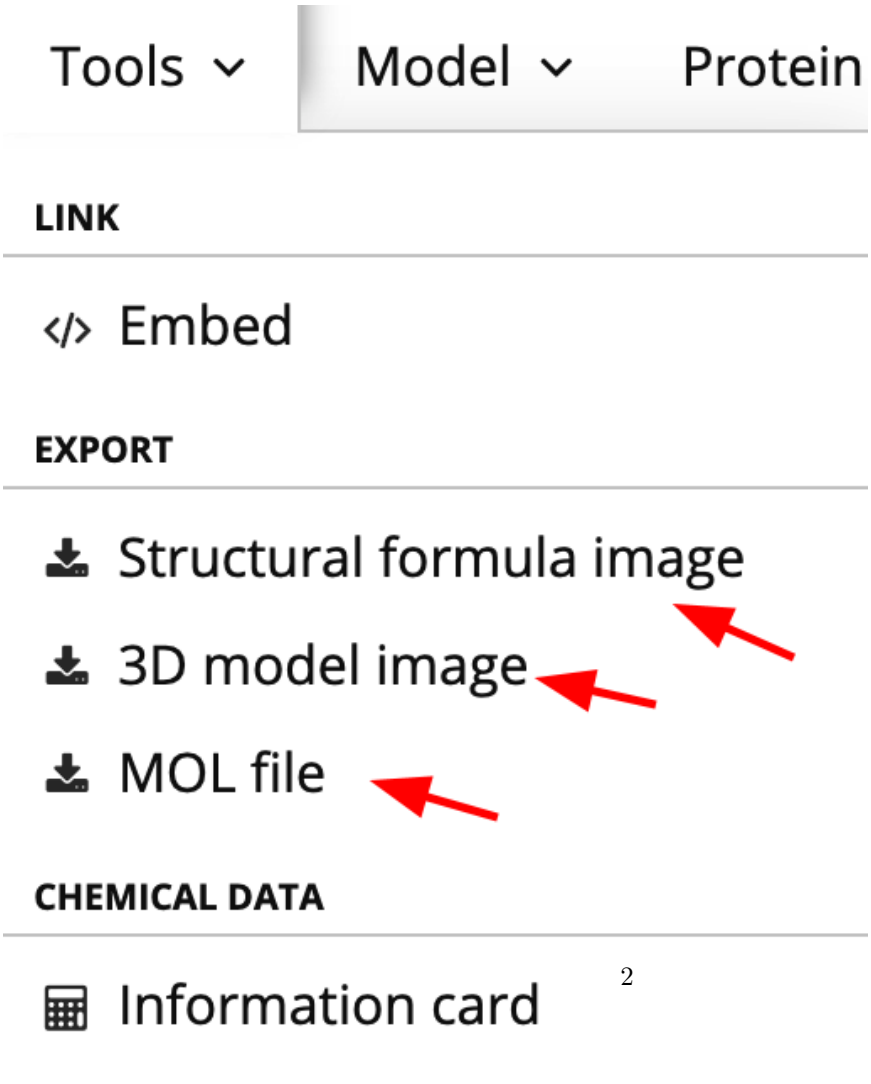


Figure 1: Toluene Example



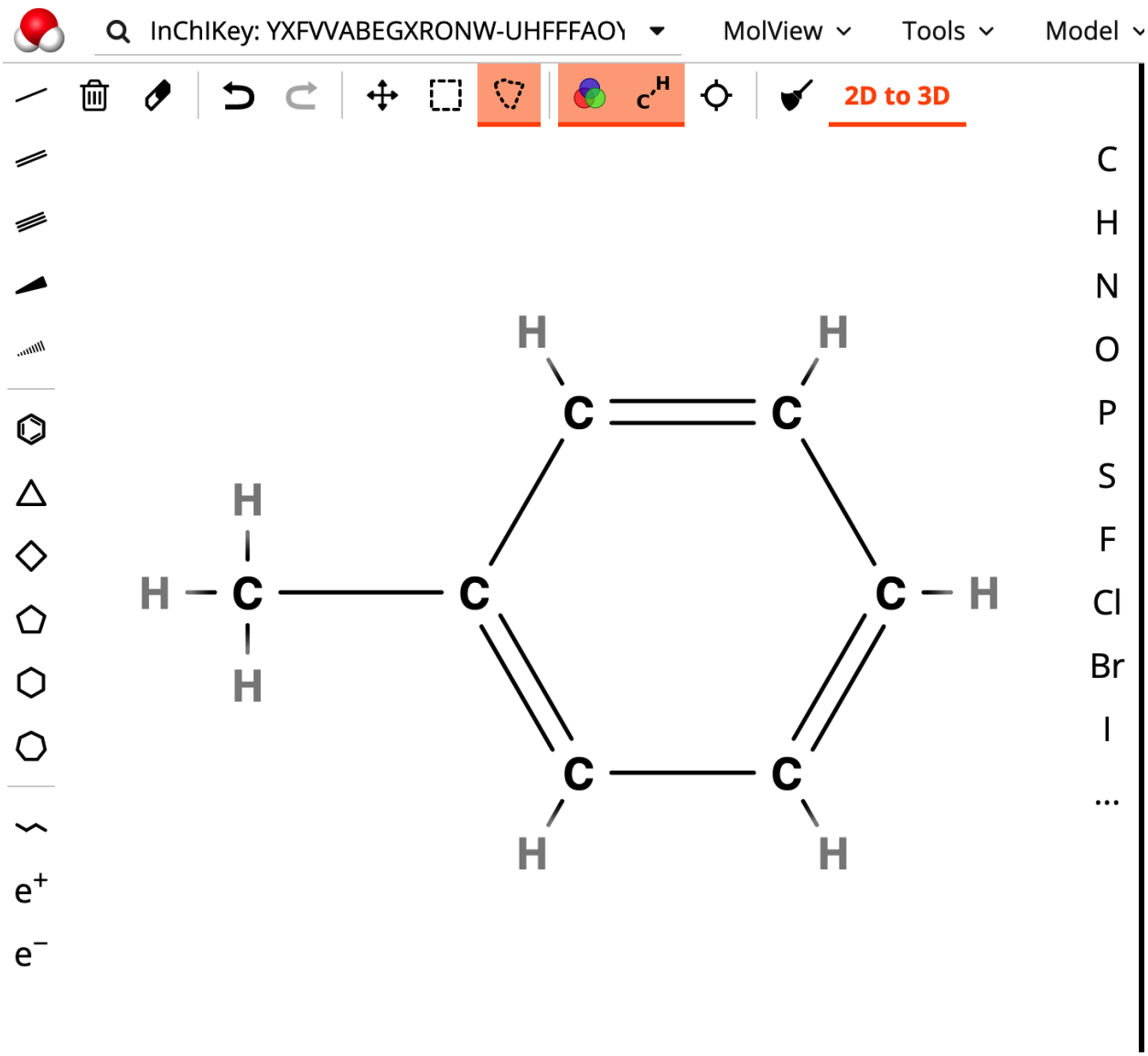


Figure 2: Toggle Bonds

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