1 Using IMES

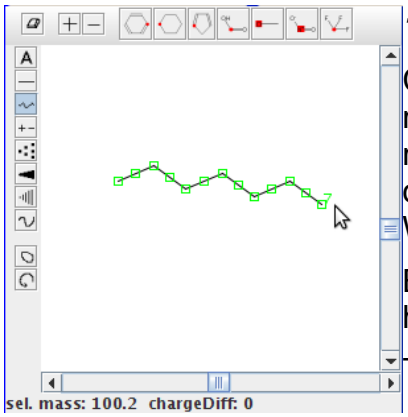

Figure 1: Chain tool

1.1 Inserting bonds

Choose the desired bond order in the left toolbar (in the simple mode, multiple bonds can be entered by clicking on a bond multiple times with the single bond tool). By clicking and dragging, you can insert bonds with a different orientation. When dragging on an existing atom, it will be connected.

By holding [Shift], you can deactivate the 15° angle lock. By holding [Ctrl], you can freely choose the bond length.

The chain tool can be used to draw alkyl chains.

1.1.1 Stereochemistry

The tool „bond up“, „bond down“ and „undefined stereochemistry“ allow to draw the respective bond types or existing single bonds can be modified.

1.2 Changing atoms

Point with the mouse cursor at an atom to be edited. If no atom is underneath the cursor, the selected atoms will be edited.

Enter an atom symbol with the keyboard, if required also with isotopic mass as prefix or followed by the number of hydrogen atoms and the charge. Moreover, it is possible to type the abbreviation of a template. In all cases, complete the input by pressing [Enter].

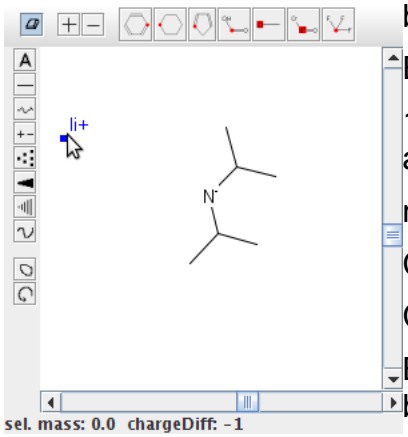

Figure 2: Entering atoms

Examples:

13C => 13-carbon atom with automatic number of hydrogen atoms

na+ => sodium ion

CH. => carbon atom with one hydrogen atom as monoradical

CH0 => carbon atom without hydrogen atoms

By pressing [Enter] without other input, the previous atom will be repeated.

For search queries, it is also possible to use the following wildcards

- % for any element
- X for halogens
- M for metal
- Ln for lanthanides

1.2.1 Charge

The charge tool allows to change an atom's charge. By clicking the left mouse button, an atom's charge is increased, the right mouse button dereases the charge. The same can be

achieved by pressing [+] or [-].

1.2.2 Radicals

The radical tool allow to increase (left mouse button) or decrease (right mouse button) the number of unpaired electrons of an atom.

1.3 Inserting templates

In the top toolbar, templates can be selected and subsequently attached to an atom or bond. The mouse wheel allows to change the attachment point within the template and the orientation.

Example: the template for 2-pyridyl is active. By attaching to a *carbon atom of benzene*, 2-phenylpyridin will be drawn. By using the mouse wheel it is also possible to draw 3- or 4-phenylpyridin. By attaching to a *bond of benzene*, it is possible to draw quinolin or iso quinolin (using the mouse wheel).

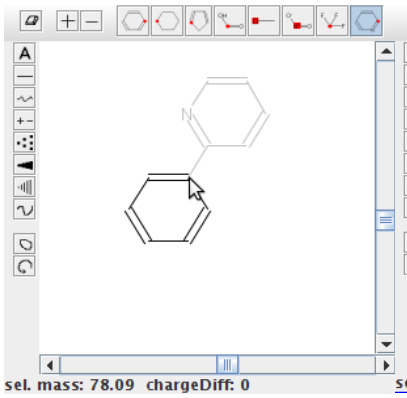

Figure 3: 2-Ph-pyridin

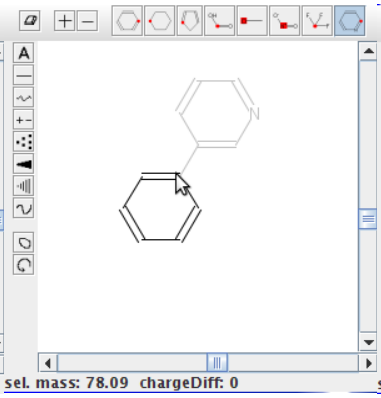

Figure 4: 3-Ph-pyridin

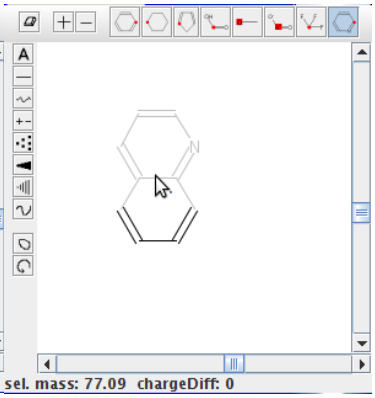

Figure 5: Quinolin

1.4 Reactions

A reaction arrow can be entered using the „-->“ tool. Components can be separated with the „+“ tool.

1.5 Structure editing

The reactangular and freehand select tools allow selecting atoms and bonds to

1. move (by dragging one of the selected atoms)
2. rotate (using the rotate tool)
3. cut/copy (by the respective toolbar buttons)
4. delete (by the respective toolbar button)

them. The mass of the selected atoms is display in the status bar.

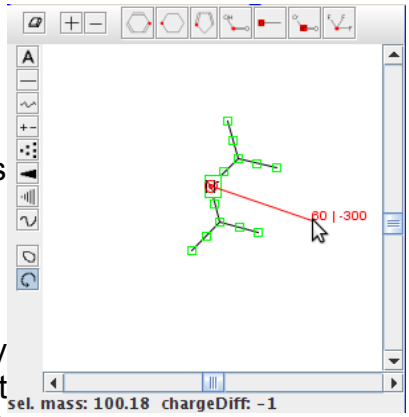

Figure 6: Rotate selection

1.5.1 Rotate

The rotate tool rotates the selection or the whole structure by dragging from the rotation center. The angle is dislpayed next to the mouse cursor, holding [Shift] deactivates the 15° angle lock.

1.5.2 Deleting atoms and bonds

By clicking or dragging with the delete tool you can remove atoms or bonds underneath the mouse cursor. Dragging with the right mouse button clears reactangular areas.

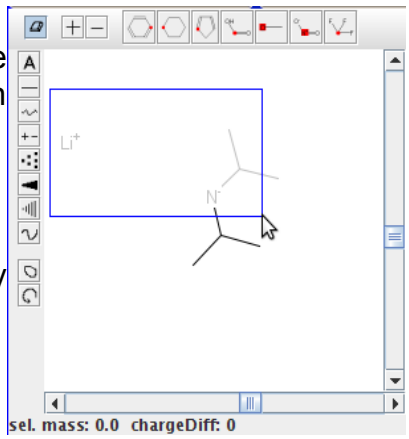

Figure 7: Delete rectangular areas

1.5.3 Undo/Redo

The respective toolbar buttons allow to move within the history of changes.

1.6 View

The toolbar buttons „+“ and „-“ zoom the view. With the scrollbars, you can navigate to different areas.

1.7 Keyboard shortcuts

[Ctrl]+X	Cut
[Ctrl]+C	Copy
[Ctrl]+V	Paste
[Del]	Delete selected atoms/bonds
[Ctrl]+Z	Undo
[Ctrl]+W	Redo