

alchemist

v0.1.4

MIT

A package to render skeletal formulas using cetz

Robotechnic <@ROBOTECHNIC>

<https://github.com/Robotechnic/alchemist>

Alchemist is a package used to draw chemical structures with skeletal formulas using Cetz. It is heavily inspired by the Chemfig package for LaTeX. This package is meant to be easy to use and customizable. It can also be used alongside the cetz package to draw more complex structures.

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Part I.

Usage

To start using Alchemist, just import the package in your document:

```
#import "@preview/alchemist:0.1.4": *
```

I.1. Initializing drawing environment

To start drawing molecules, you first need to initialise the drawing environment. This is done by calling the `#skeletonize()` function.

```
#skeletonize({  
  ...  
})
```

The main argument is a block of code that contains the drawing instructions. The block can also contain any cetz code to draw more complex structures, see Section II.7.

```
#skeletonize({debug}: false, {background}: none, {config}: (:), {body})
```

Argument

<debug>

bool

Display bounding boxes of the objects in the drawing environment.

Argument

<background>

color | none

Background color of the drawing environment

Argument

<config>

dictionary

Configuration of the drawing environment. See Section I.3.

Argument

<body>

drawable

The module to draw or any cetz drawable object.

I.2. Drawing a molecule directly in Cetz

Sometimes, you may want to draw a molecule directly in cetz. To do so, you can use the `#draw-skeleton()` function. This function is what is used internally by the `#skeletonize()` function.

```
#draw-skeleton({config}: (:), {body})
```

Argument

<config>

dictionary

Configuration of the drawing environment. See Section I.3.

1.2 Drawing a molecule directly in Cetz

Argument

`<body>`

drawable

The module to draw or any cetz drawable object.

Argument

`<name>`: `none`

If a name is provided, the molecule will be placed in a cetz group with this name.

Argument

`<mol-anchor>`: `none`

Anchor of the group. It is working the same way as the anchor argument of the cetz group function. The default anchor of the molecule is the east anchor of the first atom or the starting point of the first link.

The usefulness of this function comes when you want to draw multiples molecules in the same cetz environment. See Section II.7.

I.3. Configuration

The configuration dictionary that you can pass to `skeletize` defines a set of default values for a lot of parameters in `alchemist`.

Argument

`<atom-sep>`: `3em`

length

It defines the distance between each atom center. It is overridden by the `atom-sep` argument of `link`

Argument

`<angle-increment>`: `45deg`

angle

It defines the angle added by each increment of the `angle` argument of `link`

Argument

`<base-angle>`: `0deg`

angle

Default angle at which a link with no angle defined will be.

Argument

`<molecule-margin>`: `0.2em`

length

Default space between a molecule and all its attachments (links and lewis formulae elements).

I.3.1. Link default style

The default values also contains styling arguments for the links. You can specify default `stroke`, `fill`, `dash`, etc, depending on the link type. Each link default values are in a dictionary named after the link name.

1.3 Configuration

single

Argument	Default value
stroke	luma(0%)

double

Argument	Default value
gap	0.25em
offset	"center"
offset-coeff	0.85
stroke	luma(0%)

triple

Argument	Default value
gap	0.25em
stroke	luma(0%)

filled-cram

Argument	Default value
stroke	none
fill	luma(0%)
base-length	0.8em

dashed-cram

Argument	Default value
stroke	0.05em + luma(0%)
dash-gap	0.3em
base-length	0.8em
tip-length	0.1em

lewis-single

Argument	Default value
stroke	luma(0%)
fill	luma(0%)
radius	0.1em
gap	0.25em
offset	"top"

lewis-double

Argument	Default value
stroke	luma(0%)
fill	luma(0%)
radius	0.1em
gap	0.25em

lewis-line

Argument	Default value
stroke	luma(0%)
length	0.7em

lewis-rectangle

Argument	Default value
stroke	0.08em + luma(0%)
fill	luma(100%)
height	0.7em
width	0.3em

I.4. Available commands

I.4.1. Molecule function

```
#molecule(  
  {name}: none,  
  {links}: "(:)",  
  {lewis}: "()",  
  {vertical}: false,  
  {mol}
```

) → **drawable**

Build a molecule group based on mol. Each molecule is represented as an optional count followed by a molecule name starting by a capital letter followed by an optional exponent followed by an optional indice.

```
#skeletonize({  
  molecule("H_2O")  
})
```



```
#skeletonize({  
  molecule("H^A_EF^5_4")  
})
```



It is possible to use an equation as a molecule. In this case, the splitting of the equation uses the same rules as in the string case. However, you get some advantages over the string version:

- You can use parenthesis to group elements together.
- You have no restriction about what you can put in exponent or indice.

```
#skeletonize({  
  molecule("$C(C H_3)_3$")  
})
```



Argument

<name>: none

content

The name of the molecule. It is used as the cetz name of the molecule and to link other molecules to it.

Argument

<links>: "(:)"

dictionary

The links between this molecule and previous molecules or hooks. The key is the name of the molecule or hook and the value is the link function. See Section I.4.4.

Note that the atom-sep and angle arguments are ignored

—Argument—

`<lewis>: "("`

list

The list of lewis structures to draw around the molecules. See Section I.4.5

—Argument—

`<vertical>: false`

bool

If true, the molecule is drawn vertically

```
#skeletonize({
  molecule("ABCD", vertical: true)
})
```

A
B
C
D

—Argument—

`<mol>`

str | equation

The string representing the molecule or an equation of the molecule

I.4.2. Hooks

`#hook(<name>)` → **drawable**

Create a hook in the molecule. It allows to connect links to the place where the hook is. Hooks are placed at the end of links or at the beginning of the molecule.

—Argument—

`<name>`

str

The name of the hook

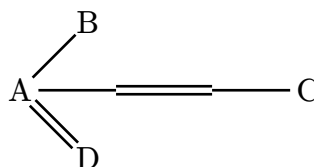
I.4.3. Branch and cycles

`#branch(..<args>)`

Create a branch from the current molecule, the first element of the branch has to be a link.

You can specify an angle argument like for links. This angle will be then used as the base-angle for the branch.

```
#skeletonize({
  molecule("A")
  branch({
    single(angle:1)
    molecule("B")
  })
  branch({
    double(angle: -1)
    molecule("D")
  })
  single()
  double()
  single()
  molecule("C")
})
```

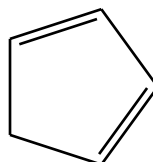


#cycle(..{args})

Create a regular cycle of molecules. You can specify an angle argument like for links. This angle will be then the angle of the first link of the cycle.

The argument `align` can be used to force align the cycle according to the relative angle of the previous link.

```
#skeletonize({
  cycle(5, {
    single()
    double()
    single()
    double()
    single()
  })
})
```



I.4.4. Link functions

I.4.4.1. Common arguments

Links functions are used to draw links between molecules. They all have the same base arguments but can be customized with additional arguments.

Argument

<angle>: 0

int

Multiplier of the angle-increment argument of the drawing environment. The final angle is relative to the abscissa axis.

Argument

<relative>: none

angle

Relative angle to the previous link. This argument override all other angle arguments.

Argument

<absolute>: none

angle

Absolute angle of the link. This argument override angle argument.

Argument

`<atom-sep>: 3em`

length

Distance between the two connected atom of the link. Default to the atom-sep entry of the configuration dictionary.

Argument

`<from>`

int

Index of the molecule in the group to start the link from. By default, it is computed depending on the angle of the link.

Argument

`<to>`

int

Index of the molecule in the group to end the link to. By default, it is computed depending on the angle of the link.

Argument

`<links>`

dictionary

Dictionary of links to other molecules or hooks. The key is the name of the molecule or the hook and the value is the link function.

1.4.4.2. Links

#build-link(*(draw-function)*) → function

Create a link function that is then used to draw a link between two points

Argument

`<draw-function>`

function

The function that will be used to draw the link. It should takes four arguments: the length of the link, the alchemist context, the cetz context, and a dictionary of named arguments that can be used to configure the links

#single

Draw a single line between two molecules

```
#skeletonize({
  molecule("A")
  single()
  molecule("B")
})
```

A — B

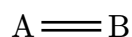
It is possible to change the color and width of the line with the stroke argument


```
#skeletalize({
  molecule("A")
  single(stroke: red + 5pt)
  molecule("B")
})
```

**#double**

Draw a double line between two molecules

```
#skeletalize({
  molecule("A")
  double()
  molecule("B")
})
```



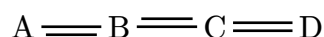
It is possible to change the color and width of the line with the `stroke` argument and the gap between the two lines with the `gap` argument

```
#skeletalize({
  molecule("A")
  double(
    stroke: orange + 2pt,
    gap: .8em
  )
  molecule("B")
})
```



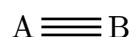
This link also supports an `offset` argument that can be set to `left`, `right` or `center`. It allows to make either the left side, right side or the center of the double line to be aligned with the link point.

```
#skeletalize({
  molecule("A")
  double(offset: "right")
  molecule("B")
  double(offset: "left")
  molecule("C")
  double(offset: "center")
  molecule("D")
})
```

**#triple**

Draw a triple line between two molecules

```
#skeletalize({
  molecule("A")
  triple()
  molecule("B")
})
```



It is possible to change the color and width of the line with the `stroke` argument and the gap between the three lines with the `gap` argument

```
#skeletalize({
  molecule("A")
  triple(
    stroke: blue + .5pt,
    gap: .15em
  )
  molecule("B")
})
```

**#cram-filled-right**

Draw a filled cram between two molecules with the arrow pointing to the right

```
#skeletalize({
  molecule("A")
  cram-filled-right()
  molecule("B")
})
```



It is possible to change the stroke and fill color of the arrow with the `stroke` and `fill` arguments. You can also change the base length of the arrow with the `base-length` argument

```
#skeletalize({
  molecule("A")
  cram-filled-right(
    stroke: red + 2pt,
    fill: green,
    base-length: 2em
  )
  molecule("B")
})
```

**#cram-filled-left**

Draw a filled cram between two molecules with the arrow pointing to the left

```
#skeletalize({
  molecule("A")
  cram-filled-left()
  molecule("B")
})
```



It is possible to change the stroke and fill color of the arrow with the `stroke` and `fill` arguments. You can also change the base length of the arrow with the `base-length` argument

```
#skeletalize({
  molecule("A")
  cram-filled-left(
    stroke: red + 2pt,
    fill: green,
    base-length: 2em
  )
  molecule("B")
})
```

**#cram-hollow-right**

Draw a hollow cram between two molecules with the arrow pointing to the right It is a shorthand for `cram-filled-right(fill: none)`

#cram-hollow-left

Draw a hollow cram between two molecules with the arrow pointing to the left It is a shorthand for `cram-filled-left(fill: none)`

#cram-dashed-right

```
#skeletalize({
  molecule("A")
  cram-dashed-right(
    stroke: red + 2pt,
    base-length: 2em,
    tip-length: 1em,
    dash-gap: .5em
  )
  molecule("B")
})
```

**#cram-dashed-left**

Draw a dashed cram between two molecules with the arrow pointing to the left

```
#skeletalize({
  molecule("A")
  cram-dashed-left()
  molecule("B")
})
```



It is possible to change the stroke of the lines in the arrow with the `stroke` argument. You can also change the base length of the arrow with the `base-length` argument and distance between the dashes with the `dash-gap` argument

```
#skeletalize({
  molecule("A")
  cram-dashed-left(
    stroke: red + 2pt,
    base-length: 2em,
    dash-gap: .5em
  )
  molecule("B")
})
```



I.4.5. Lewis structures

All the lewis elements have two common arguments to control their position:

Argument	
<code><angle></code> : 0deg	angle
Angle of the lewis element relative to the abscissa axis.	

Argument	
<code><molecule-margin></code> : 0.2em	length
Space between the lewis element and the molecule.	

`#build-lewis`(`(draw-function)`) → `function`

Create a lewis function that is then used to draw a lewis formulae element around the molecule

Argument	
<code><draw-function></code>	function
The function that will be used to draw the lewis element. It should takes three arguments: the alchemist context, the cetz context, and a dictionary of named arguments that can be used to configure the links	

`#lewis-single`

draw a sigle electron around the molecule

It is possible to change the distance from the center of the electron with the `gap` argument.

The position of the electron is set by the `offset` argument. Available values are:

- “top”: the electron is placed above the molecule center line
- “bottom”: the electron is placed below the molecule center line
- “center”: the electron is placed at the molecule center line

It is also possible to change the `radius`, `stroke` and `fill` arguments

```
#skelsize({
  molecule("A", lewis:(
    lewis-single(offset: "top"),
  ))
  single(angle:-2)
  molecule("B", lewis:(
    lewis-single(offset:
"bottom"),
  ))
  single(angle:-2)
  molecule("C", lewis:(
    lewis-single(offset:
"center"),
  ))
})
```



`#lewis-double`

Draw a pair of electron around the molecule

1.4 Available commands

It is possible to change the distance from the center of the electron with the `gap` argument. It is also possible to change the `radius`, `stroke` and `fill` arguments

```
#skeletalize({  
  molecule("A", lewis:(  
    lewis-double(),  
    lewis-double(angle: 90deg),  
    lewis-double(angle: 180deg),  
    lewis-double(angle: -90deg)  
  ))  
})
```



#lewis-line

Draw a pair of electron liked by a single line

It is possible to change the length of the line with the `length` argument. It is also possible to change the `stroke` agument

```
#skeletalize({  
  molecule("B", lewis:(  
    lewis-line(angle: 45deg),  
    lewis-line(angle: 135deg),  
    lewis-line(angle: -45deg),  
    lewis-line(angle: -135deg)  
  ))  
})
```



#lewis-rectangle

Draw a rectangle to denote a lone pair of electrons

It is possible to change the height and width of the rectangle with the `height` and `width` arguments. It is also possible to change the `fill` and `stroke` arguments

```
#skeletalize({  
  molecule("C", lewis:(  
    lewis-rectangle(),  
    lewis-rectangle(angle: 180deg)  
  ))  
})
```



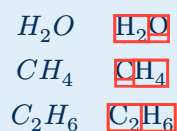
Part II.

Drawing molecules

II.1. Atoms

In alchemist, the name of the function `#molecule()` is used to create a group of atom but here it is a little bit abusive as it do not necessarily represent real molecules. An atom is in our case something of the form: optional number + capital letter + optional lowercase letter followed by indices or exponent.

For instance, H_2O is a molecule of the atoms H_2 and O . If we look at the bounding boxes of the molecules, we can see that separation.



This separation does not have any impact on the drawing of the molecules but it will be useful when we will draw more complex structures.

II.2. Links

There are already som links available with the package (see Section I.4.4) and you can create your own links with the `#build-link()` function but they all share the same base arguments used to control their behaviors.

II.2.1. Atom separation

Each atom is separated by a distance defined by the `atom-sep` argument of the drawing environment. This distance can be overridden by the `atom-sep` argument of the link. It defines the distance between the center of the two connected atoms.

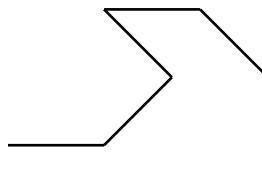
The behavior is not well defined yet.

II.2.2. Angle

There are three ways to define the angle of a link: using the `angle` argument, the `relative` argument, or the `absolute` argument.

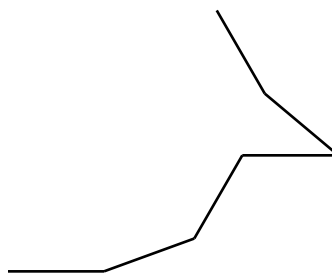
The argument `angle` is a multiplier of the `angle-increment` argument.

```
#skeletonize({
  single()
  single(angle:1)
  single(angle:3)
  single()
  single(angle:7)
  single(angle:6)
})
```



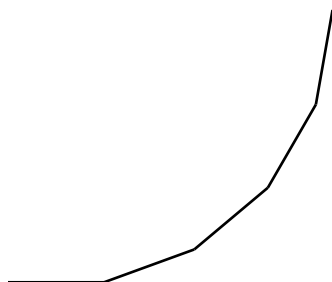
Changing the angle-increment argument of the drawing environment will change the angle of the links.

```
#skeletonize(config:(angle-
  increment:20deg),{
  single()
  single(angle:1)
  single(angle:3)
  single()
  single(angle:7)
  single(angle:6)
})
```



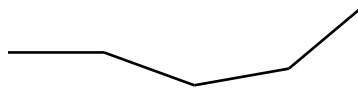
The argument `relative` allows you to define the angle of the link relative to the previous link.

```
#skeletonize({
  single()
  single(relative:20deg)
  single(relative:20deg)
  single(relative:20deg)
  single(relative:20deg)
})
```



The argument `absolute` allows you to define the angle of the link relative to the abscissa axis.

```
#skeletonize({
  single()
  single(absolute:-20deg)
  single(absolute:10deg)
  single(absolute:40deg)
  single(absolute:-90deg)
})
```

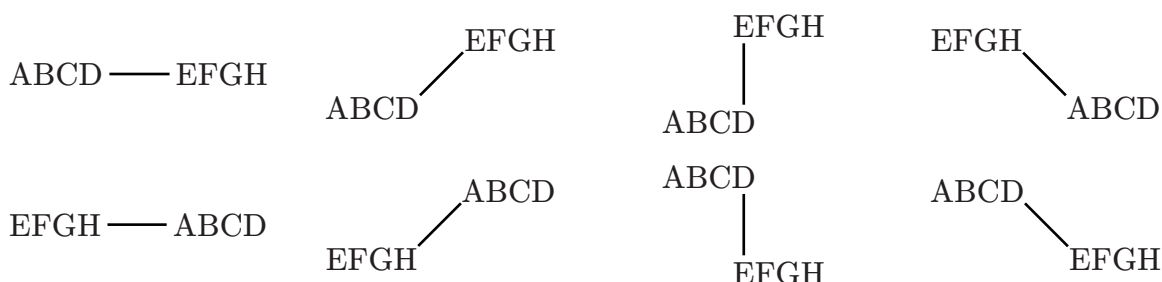


II.2.3. Starting and ending points

By default, the starting and ending points of the links are computed depending on the angle of the link. You can override this behavior by using the `from` and `to` arguments.

If the angle is in $] - 90 \text{ deg}; 90 \text{ deg}]$, the starting point is the last atom of the previous molecule and the ending point is the first atom of the next molecule. If the angle is in $]90 \text{ deg}; 270 \text{ deg}]$, the starting point is the first atom of the previous molecule and the ending point is the last atom of the next molecule.

2.2 Links



If you choose to override the starting and ending points, you can use the `from` and `to` arguments. The only constraint is that the index must be in the range $[0, n - 1]$ where n is the number of atoms in the molecule.



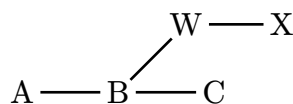
The fact that you can chose any index for the `from` and `to` arguments can lead to some weird results. Alchemist can't check if he result is beautiful or not.

II.3. Branches

Drawing linear molecules is nice but being able to draw molecule with branches is even better. To do so, you can use the `#branch()` function.

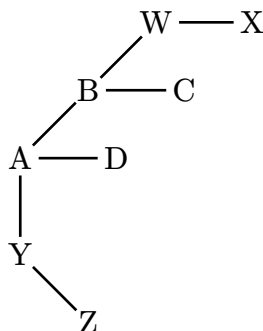
The principle is simple. When you draw normal molecules, each time an element is added, the attachment point is moved accordingly to the added object. Drawing a branch is a way to tell alchemist that you want the attachment point to say the same for the others elements outside the branch. The only constraint is that the branch must start with a link.

```
#skeletonize({  
  molecule("A")  
  single()  
  molecule("B")  
  branch({  
    single(angle:1)  
    molecule("W")  
    single()  
    molecule("X")  
  })  
  single()  
  molecule("C")  
})
```



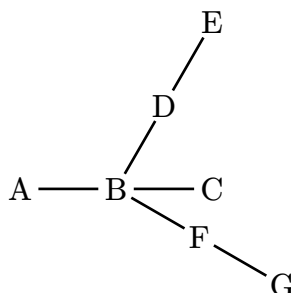
It is of course possible to have nested branches or branches with the same starting point.


```
#skeletonize({
  molecule("A")
  branch({
    single(angle:1)
    molecule("B")
    branch({
      single(angle:1)
      molecule("W")
      single()
      molecule("X")
    })
    single()
    molecule("C")
  })
  branch({
    single(angle:-2)
    molecule("Y")
    single(angle:-1)
    molecule("Z")
  })
  single()
  molecule("D")
})
```



You can also specify an angle argument like for links. This angle will be then used as the base-angle for the branch. It means that all the links with no angle defined will be drawn with this angle.

```
#skeletonize({
  molecule("A")
  single()
  molecule("B")
  branch(relative:60deg,{
    single()
    molecule("D")
    single()
    molecule("E")
  })
  branch(relative:-30deg,{
    single()
    molecule("F")
    single()
    molecule("G")
  })
  single()
  molecule("C")
})
```



II.4. Link distant atoms

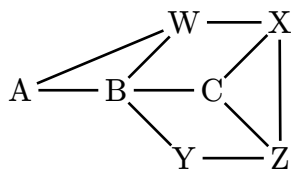
II.4.1. Basic usage

From then, the only way to link atoms is to use links functions and putting them one after the other. This doesn't allow to do cycles or to link atoms that are not next to each other in the code. The way alchemist handle this is with the `links` and `name` arguments of the `#molecule()` function.

```

#skeletalize({
  molecule(name: "A", "A")
  single()
  molecule("B")
  branch({
    single(angle: 1)
    molecule(
      "W",
      links: (
        "A": single(),
      ),
    )
    single()
    molecule(name: "X", "X")
  })
  branch({
    single(angle: -1)
    molecule("Y")
    single()
    molecule(
      name: "Z",
      "Z",
      links: (
        "X": single(),
      ),
    )
  })
  single()
  molecule(
    "C",
    links: (
      "X": single(),
      "Z": single(),
    ),
  )
})

```



In this example, we can see that the molecules are linked to the molecules defined before with the name argument. Note that you can't link to a molecule that is defined after the current one because the name is not defined yet. It's a limitation of the current implementation.

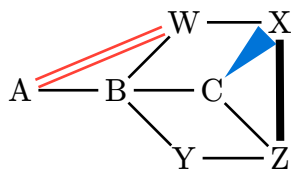
II.4.2. Customizing links

If you look at the previous example, you can see that the links used in the `links` argument are functions. This is because you can still customize the links as you want. The only thing that is not taken into account are the `length` and `angle` arguments. It means that you can change color, from and to arguments, etc.

```

#skeletonize({
  molecule(name: "A", "A")
  single()
  molecule("B")
  branch({
    single(angle: 1)
    molecule(
      "W",
      links: (
        "A": double(stroke: red),
      ),
    )
    single()
    molecule(name: "X", "X")
  })
  branch({
    single(angle: -1)
    molecule("Y")
    single()
    molecule(
      name: "Z",
      "Z",
      links: (
        "X": single(stroke: black
+ 3pt),
      ),
    )
  })
  single()
  molecule(
    "C",
    links: (
      "X": cram-filled-left(fill:
blue),
      "Z": single(),
    ),
  )
})

```



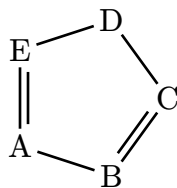
II.5. Cycles

II.5.1. Basic usage

Using branches and links arguments, you can draw cycles. However, depending on the number of faces, the angle calculation is fastidious. To help you with that, you can use the `#cycle()` function.

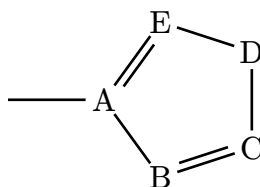
The default behavior if the angle is 0 deg is to be placed in a way that the last link is vertical.

```
#skeletonize({
  molecule("A")
  cycle(5, {
    single()
    molecule("B")
    double()
    molecule("C")
    single()
    molecule("D")
    single()
    molecule("E")
    double()
  })
})
```



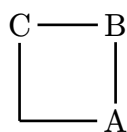
If the angle is not 0 deg or if the align argument is set, the cycle will be drawn in relation with the relative angle of the last link.

```
#skeletonize({
  single()
  molecule("A")
  cycle(5, align: true, {
    single()
    molecule("B")
    double()
    molecule("C")
    single()
    molecule("D")
    single()
    molecule("E")
    double()
  })
})
```



A cycle must start by a link and if there is more links than the number of faces, the excess links will be ignored. Nevertheless, it is possible to have less links than the number of faces.

```
#skeletonize({
  cycle(4, {
    single()
    molecule("A")
    single()
    molecule("B")
    single()
    molecule("C")
    single()
    molecule("D")
  })
})
```



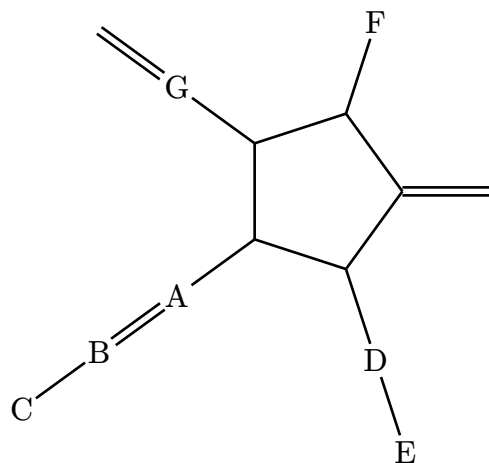
II.5.2. Branches in cycles

It is possible to add branches in cycles. You can add a branch at any point of the cycle. The default angle of the branch will be set in a way that it is the bisector of the two links that are next to the branch.

```

#skeletonize({
  cycle(5,{
    branch({
      single()
      molecule("A")
      double()
      molecule("B")
      single()
      molecule("C")
    })
    single()
    branch({
      single()
      molecule("D")
      single()
      molecule("E")
    })
    single()
    branch({
      double()
    })
    single()
    branch({
      single()
      molecule("F")
    })
    single()
    branch({
      single()
      molecule("G")
      double()
    })
    single()
    single()
    single()
    single()
  })
})

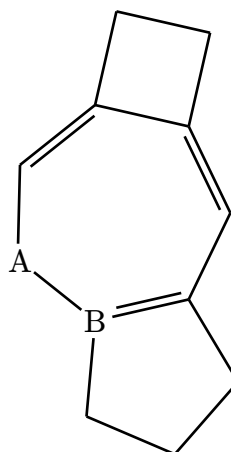
```



II.5.3. Cycles imbrication

Like branches, you can add cycles in cycles. By default the cycle will be placed in a way that the two cycles share a common link.

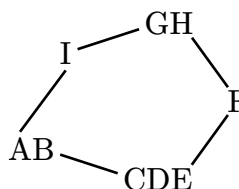
```
#skeletonize({
  molecule("A")
  cycle(7,{
    single()
    molecule("B")
    cycle(5,{
      single()
      single()
      single()
      single()
    })
    double()
    single()
    double()
    cycle(4,{
      single()
      single()
      single()
    })
    single()
    double()
    single()
  })
})
```



II.5.4. Issues with atom groups

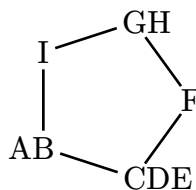
Cycles by default have an issue with atom groups with multiples atoms. The links are not well placed for the cycle to be drawn correctly.

```
#skeletonize({
  molecule("AB")
  cycle(5,{
    single()
    molecule("CDE")
    single()
    molecule("F")
    single()
    molecule("GH")
    single()
    molecule("I")
    single()
  })
})
```



To fix that, you have to use the `from` and `to` arguments of the links to specify the starting and ending points of the links.

```
#skeletalize({
  molecule("AB")
  cycle(5, {
    single(from: 1, to: 0)
    molecule("CDE")
    single(from: 0)
    molecule("F")
    single(to: 0)
    molecule("GH")
    single(from: 0)
    molecule("I")
    single(to: 1)
  })
})
```



II.5.5. Arcs

It is possible to draw arcs in cycles. The arc argument is a dictionary with the following entries:

Argument

<start>: 0deg

angle

Angle at which the arc starts.

Argument

<end>: 360deg

angle

Angle at which the arc ends.

Argument

<delta>: none

angle

Angle of the arc in degrees.

Argument

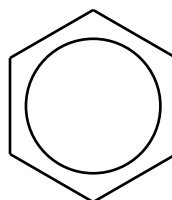
<radius>: none

float

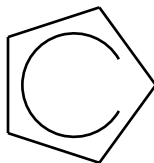
Radius of the arc in percentage of the smallest distance between two opposite atoms in the cycle. By default, it is set to 0.7 for cycle with more than 4 faces and 0.5 for cycle with 4 or 3 faces.

Any styling argument of the cetz arc function can be used.

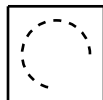
```
#skeletalize({
  cycle(6, arc:(:), {
    single()
    single()
    single()
    single()
    single()
    single()
  })
})
```



```
#skeletonize({
  cycle(5, arc:(start: 30deg, end:
330deg), {
    single()
    single()
    single()
    single()
    single()
  })
})
```



```
#skeletonize({
  cycle(4, arc:(start: 0deg, delta:
270deg, stroke: (paint: black, dash:
"dashed")), {
    single()
    single()
    single()
    single()
  })
})
```



II.6. Custom links

Using the `#build-link()` function, you can create your own links. The function passed as argument to `#build-link()` must takes four arguments:

- The length of the link
- The alchemist context
- The cetz context of the drawing environment
- A dictionary of named arguments that can be used to configure the links

You can then draw anything you want using the cetz functions. For instance, here is the code for the single link:

```
#let single = build-link((length, ctx, _, args) => {
  import cetz.draw: *
  line((0, 0), (length, 0), stroke: args.at("stroke", default:
ctx.config.single.stroke))
})
```

II.7. Integration with cetz

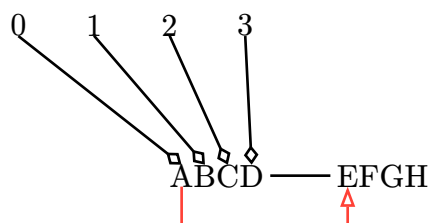
II.7.1. Molecules

If you name your molecules with the name argument, you can use them in cetz code. The name of the molecule is the name of the cetz object. Accessing to atoms is done by using the anchors numbered by the index of the atom in the molecule.


```

#skeletonize({
  import cetz.draw: *
  molecule("ABCD", name: "A")
  single()
  molecule("EFGH", name: "B")
  line(
    "A.0.south",
    (rel: (0, -0.5)),
    (to: "B.0.south", rel: (0, -0.5)),
    "B.0.south",
    stroke: red,
    mark: (end: ">"),
  )
  for i in range(0, 4) {
    content((-2 + i, 2), $#i$, name: "label-" + str(i))
    line(
      (name: "label-" + str(i), anchor: "south"),
      (name: "A", anchor: (str(i), "north")),
      mark: (end: "<>"),
    )
  }
})

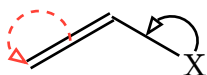
```



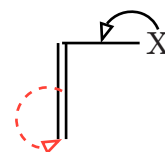
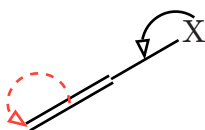
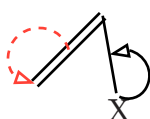
II.7.2. Links

If you name your links with the name argument, you can use them in cetz code. The name of the link is the name of the cetz object. It exposes the same anchors as the `line` function of cetz.

```
#skeletonize({
  import cetz.draw: *
  double(absolute: 30deg, name: "l1")
  single(absolute: -30deg, name: "l2")
  molecule("X", name: "X")
  hobby(
    "l1.50%",
    ("l1.start", 0.5, 90deg, "l1.end"),
    "l1.start",
    stroke: (paint: red, dash: "dashed"),
    mark: (end: ">"),
  )
  hobby(
    (to: "X.north", rel: (0, 1pt)),
    ("l2.end", 0.4, -90deg, "l2.start"),
    "l2.50%",
    mark: (end: ">"),
  )
})
```



Here, all the used coordinates for the arrows are computed using relative coordinates. It means that if you change the position of the links, the arrows will be placed accordingly without any modification.



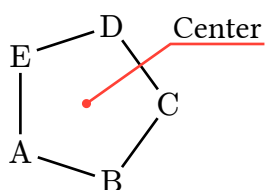
II.7.3. Cycles centers

The cycles centers can be accessed using the name of the cycle. If you name a cycle, an anchor will be placed at the center of the cycle. If the cycle is incomplete, the missing vertex will be approximated based on the last link and the atom-sep value. This will in most cases place the center correctly.

```

#skeletonize({
  import cetz.draw: *
  molecule("A")
  cycle(
    5,
    name: "cycle",
    {
      single()
      molecule("B")
      single()
      molecule("C")
      single()
      molecule("D")
      single()
      molecule("E")
      single()
    },
  )
  content(
    (to: "cycle", rel: (angle: 30deg, radius: 2)),
    "Center",
    name: "label",
  )
  line(
    "cycle",
    (to: "label.west", rel: (-1pt, -.5em)),
    (to: "label.east", rel: (1pt, -.5em)),
    stroke: red,
  )
  circle(
    "cycle",
    radius: .1em,
    fill: red,
    stroke: red,
  )
})

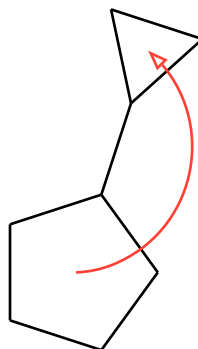
```



```

#skeletonize({
  import cetz.draw: *
  cycle(5, name: "c1", {
    single()
    single()
    single()
    branch({
      single()
      cycle(3, name: "c2", {
        single()
        single()
        single()
      })
    })
    single()
    single()
  })
  hobby(
    "c1",
    ("c1", 0.5, -60deg, "c2"),
    "c2",
    stroke: red,
    mark: (end: ">"),
  )
})

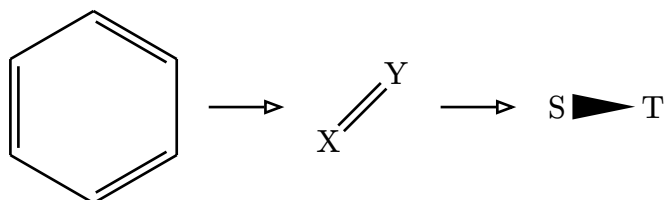
```



II.7.4. Multiple molecules

Alchemist allows you to draw multiple molecules in the same cetz environment. This is useful when you want to draw things like reactions.

```
#cetz.canvas({
  import cetz.draw: *
  draw-skeleton(name: "mol1", {
    cycle(6, {
      single()
      double()
      single()
      double()
      single()
      double()
    })
  })
  line((to: "mol1.east", rel: (1em, 0)), (rel: (1, 0)), mark: (end: ">"))
  set-origin((rel: (1em, 0)))
  draw-skeleton(name: "mol2", mol-anchor: "west", {
    molecule("X")
    double(angle: 1)
    molecule("Y")
  })
  line((to: "mol2.east", rel: (1em, 0)), (rel: (1, 0)), mark: (end: ">"))
  set-origin((rel: (1em, 0)))
  draw-skeleton(name: "mol3", {
    molecule("S")
    cram-filled-right()
    molecule("T")
  })
})
```

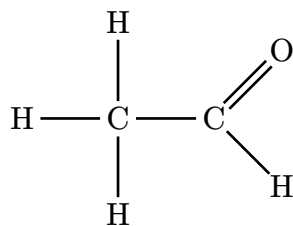


II.8. Examples

The following examples are the same ones as in the Chemfig documentation. They are here for two purposes: To show you how to draw the same structures with Alchemist and to show you how to use the package.

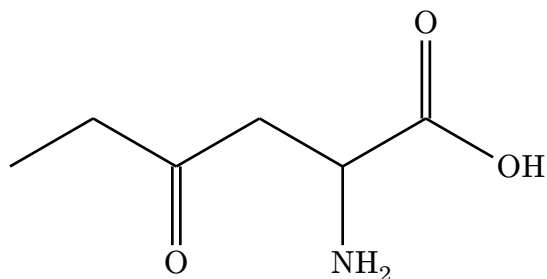
II.8.1. Ethanol

```
#skeletonize({  
  molecule("H")  
  single()  
  molecule("C")  
  branch({  
    single(angle:2)  
    molecule("H")  
  })  
  branch({  
    single(angle:-2)  
    molecule("H")  
  })  
  single()  
  molecule("C")  
  branch({  
    single(angle:-1)  
    molecule("H")  
  })  
  branch({  
    double(angle:1)  
    molecule("O")  
  })  
})
```



II.8.2. 2-Amino-4-oxohexanoic acid

```
#skeletonize(  
  config: (angle-increment: 30deg),  
  {  
    single(angle:1)  
    single(angle:-1)  
    branch({  
      double(angle:-3)  
      molecule("O")  
    })  
    single(angle:1)  
    single(angle:-1)  
    branch({  
      single(angle:-3)  
      molecule("NH_2")  
    })  
    single(angle:1)  
    branch({  
      double(angle:3)  
      molecule("O")  
    })  
    single(angle:-1)  
    molecule("OH")  
  })  
)
```

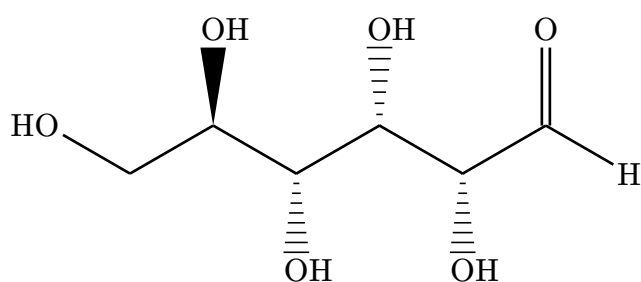


II.8.3. Glucose

```

#skeletonize(
  config: (angle-increment: 30deg),
  {
    molecule("HO")
    single(angle:-1)
    single(angle:1)
    branch({
      cram-filled-left(angle: 3)
      molecule("OH")
    })
    single(angle:-1)
    branch({
      cram-dashed-left(angle: -3)
      molecule("OH")
    })
    single(angle:1)
    branch({
      cram-dashed-left(angle: 3)
      molecule("OH")
    })
    single(angle:-1)
    branch({
      cram-dashed-left(angle: -3)
      molecule("OH")
    })
    single(angle:1)
    branch({
      double(angle: 3)
      molecule("O")
    })
    single(angle:-1)
    molecule("H")
  })

```

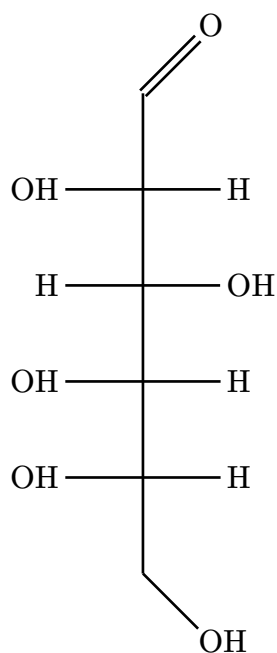


II.8.4. Fisher projection

```

#let fish-left = {
  single()
  branch({
    single(angle:4)
    molecule("H")
  })
  branch({
    single(angle:0)
    molecule("OH")
  })
}
#let fish-right = {
  single()
  branch({
    single(angle:4)
    molecule("OH")
  })
  branch({
    single(angle:0)
    molecule("H")
  })
}
#skeletonize(
  config: (base-angle: 90deg),
  {
    molecule("OH")
    single(angle:3)
    fish-right
    fish-right
    fish-left
    fish-right
    single()
    double(angle: 1)
    molecule("O")
  }
)

```

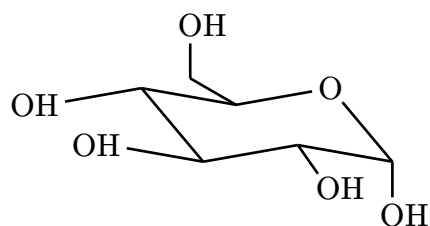


II.8.5. α -D-glucose

```

#skeletonize({
  hook("start")
  branch({
    single(absolute: 190deg)
    molecule("OH")
  })
  single(absolute: -50deg)
  branch({
    single(absolute: 170deg)
    molecule("OH")
  })
  single(absolute: 10deg)
  branch({
    single(
      absolute: -55deg,
      atom-sep: 0.7
    )
    molecule("OH")
  })
  single(absolute: -10deg)
  branch({
    single(angle: -2, atom-sep: 0.7)
    molecule("OH")
  })
  single(absolute: 130deg)
  molecule("O")
  single(absolute: 190deg, links:
("start": single()))
  branch({
    single(
      absolute: 150deg,
      atom-sep: 0.7
    )
    single(angle: 2, atom-sep: 0.7)
    molecule("OH")
  })
})

```

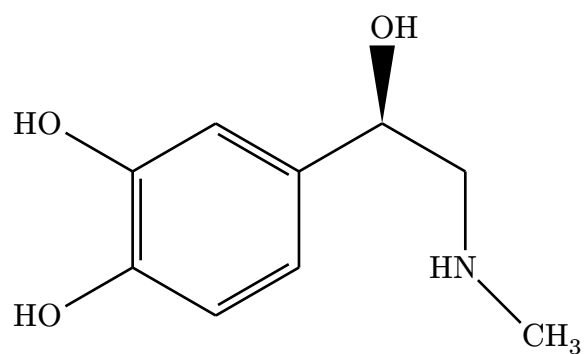


II.8.6. Adrenaline

```

#skeletonize({
  cycle(6, {
    branch({
      single()
      molecule("HO")
    })
    single()
    double()
    cycle(6, {
      single(stroke:transparent)
      single(
        stroke:transparent,
        to: 1
      )
      molecule("HN")
      branch({
        single(angle:-1)
        molecule("CH_3")
      })
      single(from:1)
      single()
      branch({
        cram-filled-left(angle: 2)
        molecule("OH")
      })
      single()
    })
    single()
    double()
    single()
    branch({
      single()
      molecule("HO")
    })
    double()
  })
})

```

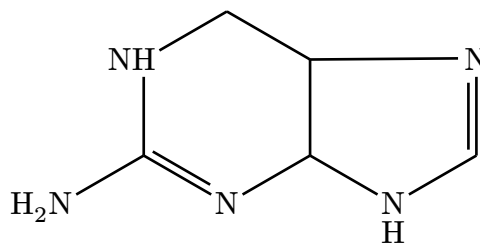


II.8.7. Guanine

```

#skeletonize({
  cycle(6, {
    branch({
      single()
      molecule("H_2N")
    })
    double()
    molecule("N")
    single()
    cycle(6, {
      single()
      molecule("NH", vertical: true)
      single()
      double()
      molecule("N", links: {
        "N-horizon": single()
      })
    })
    single()
    hook("N-horizon")
    single()
    single()
    molecule("NH")
    single(from: 1)
  })
})

```

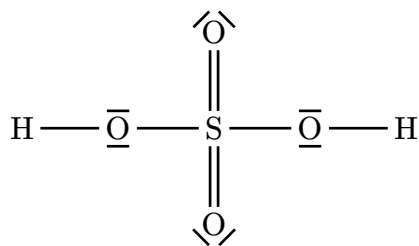


II.8.8. Sulfuric Acid

```

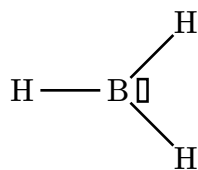
#skeletonize({
  molecule("H")
  single()
  molecule("O", lewis: (
    lewis-line(angle: 90deg),
    lewis-line(angle: -90deg)
  ))
  single()
  molecule("S")
  branch(angle: 2, {
    double()
    molecule("O", lewis: (
      lewis-line(angle: 45deg),
      lewis-line(angle: 135deg)
    ))
  })
  branch(angle: -2, {
    double()
    molecule("O", lewis: (
      lewis-line(angle: -45deg),
      lewis-line(angle: -135deg)
    ))
  })
  single()
  molecule("O", lewis: (
    lewis-line(angle: 90deg),
    lewis-line(angle: -90deg)
  ))
  single()
  molecule("H")
})

```



II.8.9. BH_3

```
#skeletalize({  
  molecule("H")  
  single()  
  molecule("B", lewis: (  
    lewis-rectangle(molecule-margin:  
5pt),  
  ))  
  branch(angle:1, {  
    single()  
    molecule("H")  
  })  
  branch(angle:-1, {  
    single()  
    molecule("H")  
  })  
})
```



Part III.

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