The "alchemist" package

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A package to render skeletal formulas using CeTZ

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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:0.1.6": *
```

I.1 Initializing drawing environment

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

```
#skeletize({
  ...
})
```

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.

`#skeletize((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 `#skeletize` function.

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

Argument
`⟨config⟩` `dictionary`

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

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
`⟨fragment-margin⟩: 0.2em` `length`

Default space between a molecule and all it's attachements (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.

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

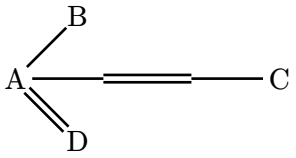
#branch(⟨body⟩, ..⟨args⟩) → drawable

I.4.1 Branch and cycles

Create a branch from the current fragment, 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.

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



Argument

⟨body⟩ drawable

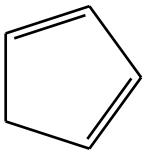
the body of the branch. It must start with a link.

#cycle(⟨faces⟩, ⟨body⟩, ..⟨args⟩) → drawable

Create a regular cycle of fragments 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.

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



Argument

⟨faces⟩ `int`

the number of faces of the cycle

Argument

⟨body⟩ `drawable`

the body of the cycle. It must start and end with a fragment or a link.

```
#fragment(
  ⟨mol⟩,
  ⟨name⟩: none,
  ⟨links⟩: (:),
  ⟨lewis⟩: (),
  ⟨vertical⟩: false,
  ⟨colors⟩: none
) → drawable
```

I.4.2 Fragment function

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

```
#skeletize({
  fragment("H_2O")
})
```

H_2O

```
#skeletize({
  fragment("H^A_EF^5_4")
})
```

$$\mathrm{H_E^AF_4^5}$$

It is possible to use an equation as a fragment. 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.

```
#skeletize({
  fragment($C(C H_3)_3$)
})
```

$$\mathrm{C(CH_3)_3}$$

Argument

⟨mol⟩ `str` | `equation`

The string representing the fragment or an equation of the fragment

Argument

⟨name⟩: none `content`

The name of the fragment. It is used as the cetz name of the fragment and to link other fragments to it.

Argument

⟨links⟩: (:) `dictionary`

The links between this fragment and previous fragments or hooks. The key is the name of the fragment or hook and the value is the link function. See Section I.4.5.

Note that the atom-sep and angle arguments are ignored

Argument

⟨lewis⟩: () `list`

The list of lewis structures to draw around the fragments. See Section I.4.6

Argument

⟨vertical⟩: false `bool`

If true, the fragment is drawn vertically

- colors (color|list): The color of the fragment. If a list is provided, it colors each group of the fragment with the corresponding color from right to left. If the number of colors

is less than the number of groups, the last color is used for the remaining groups. If the number of colors is greater than the number of groups, the extra colors are ignored.

```
#skeletize({
  fragment("ABCD", vertical: true)
})
```

A
B
C
D

#hook(⟨name⟩) → drawable

I.4.3 Hooks

Create a hook in the fragment. 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 fragment.

Argument

⟨name⟩ `str`

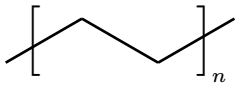
The name of the hook

```
#parenthesis(
  ⟨body⟩,
  ⟨l⟩: "(",
  ⟨r⟩: ")",
  ⟨align⟩: true,
  ⟨height⟩: none,
  ⟨yoffset⟩: none,
  ⟨xoffset⟩: none,
  ⟨right⟩: none,
  ⟨tr⟩: none,
  ⟨br⟩: none
) → drawable
```

I.4.4 Parenthesis

Encapsulate a drawable between two parenthesis. The left parenthesis is placed at the left of the first element of the body and by default the right parenthesis is placed at the right of the last element of the body.

```
#skeletize(
  config: (
    angle-increment: 30deg
  ), {
  parenthesis(
    l:"[", r:"]",
    br: $n$, {
    single(angle: 1)
    single(angle: -1)
    single(angle: 1)
  })
})
```



For more examples, see Section II.8

Argument

⟨body⟩ `drawable`

the body of the parenthesis. It must start and end with a fragment or a link.

Argument

⟨l⟩: "(" `str`

the left parenthesis

Argument

⟨r⟩: ")" `str`

the right parenthesis

Argument

⟨align⟩: true `true`

if true, the parenthesis will have the same y position. They will also get sized and aligned according to the body height. If false, they are not aligned and the height argument must be specified.

Argument

⟨height⟩: none `float` | `length`

the height of the parenthesis. If align is true, this argument is optional.

Argument

⟨yoffset⟩: none `float` | `length` | `list`

the vertical offset of parenthesis. You can also provide a tuple for left and right parenthesis

Argument
`(xoffset): none` `float` | `length` | `list`

the horizontal offset of parenthesis. You can also provide a tuple for left and right parenthesis

Argument
`(right): none` `str`

Sometime, it is not convenient to place the right parenthesis at the end of the body. In this case, you can specify the name of the fragment or link where the right parenthesis should be placed. It is especially useful when the body end by a cycle. See Section II.8.11

Argument
`(tr): none` `content`

the exponent content of the right parenthesis

Argument
`(br): none` `content`

the indice content of the right parenthesis

I.4.5 Link functions

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
`(antom-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.

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 fragments

```
#skeletize({
  fragment("A")
  single()
  fragment("B")
})
```

A —— B

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

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

#double

Draw a double line between two fragments

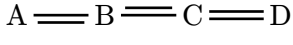
```
#skeletize({
  fragment("A")
  double()
  fragment("B")
})
```

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

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

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

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



#triple

Draw a triple line between two fragments

```
#skeletize({
  fragment("A")
  triple()
  fragment("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

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

#cram-filled-right

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

```
#skeletize({
  fragment("A")
  cram-filled-right()
  fragment("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

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

#cram-filled-left

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

```
#skeletize({
  fragment("A")
  cram-filled-left()
  fragment("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

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

#cram-hollow-right

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

#cram-dashed-right

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

#cram-dashed-left

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

```
#skeletize({
  fragment("A")
  cram-dashed-left()
  fragment("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

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

I.4.6 Lewis structures

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

Argument

`⟨angle⟩: 0deg` `angle`

Angle of the lewis element relative to the abscissa axis.

Argument

`⟨fragment-margin⟩: 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 fragment

Argument

`⟨draw-function⟩` `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 fragment

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 fragment center line
- “bottom”: the electron is placed below the fragment center line
- “center”: the electron is placed at the fragment center line

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

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

#lewis-double

Draw a pair of electron around the fragment

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

```
#skeletize({
  fragment("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 `lenght` argument. It is also possible to change the `stroke` agument

```
#skeletize({
  fragment("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

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

Part II
Drawing molecules

II.1 Atoms

In alchemist, the name of the function `#fragment` is used to create a group of atom in a molecule. A fragment is in our case something of the form: optional number + capital letter + optional lowercase letter optionally followed by a charge, an exponent or a subscript.

> 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.
>
> H_2O 
> CH_4 
> C_2H_6 
> R'^2 

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.4.5) 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.

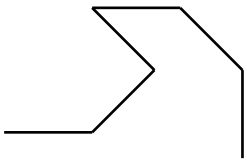
The behavior is not well defined yet.

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.

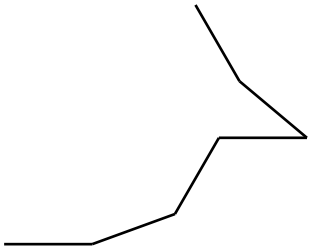
The argument `angle` is a multiplier of the `angle-increment` argument.

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



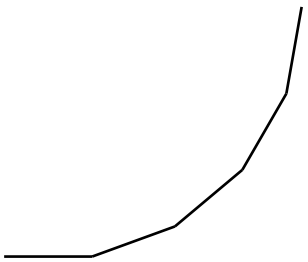
Changing the `angle-increment` argument of the drawing environment will change the angle of the links.

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



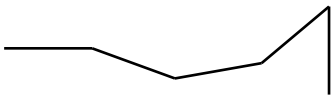
The argument `relative` allows you to define the angle of the link relative to the previous link.

```
#skeletize({
  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.

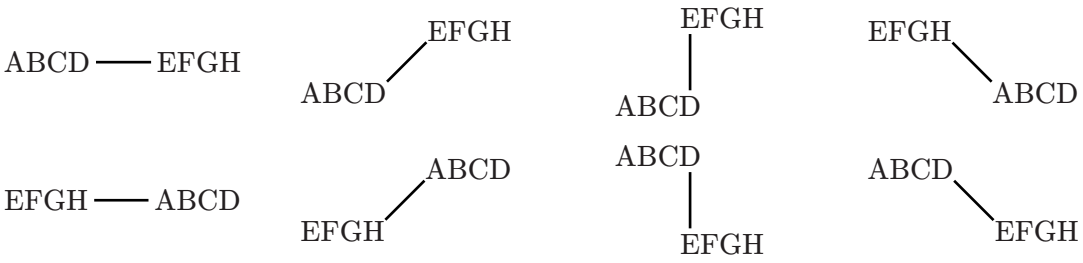
```
#skeletize({
  single()
  single(absolute:-20deg)
  single(absolute:10deg)
  single(absolute:40deg)
  single(absolute:-90deg)
})
```



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.



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.

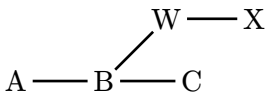
> The fact that you can chose any index for the `from` and `to` arguments can lead to some weird results. Alchemist can't check if he result is beautiful or not.

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.

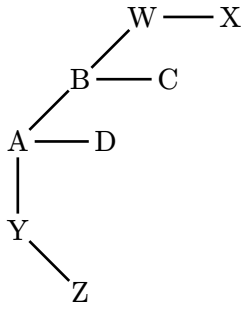
The principle is simple. When you draw normal molecules, each time an element is added, the attachement point is moved accordingly to the added object. Drawing a branch is a way to tell alchemist that you want the attachement point to say the same for the others elements outside the branch. The only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

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



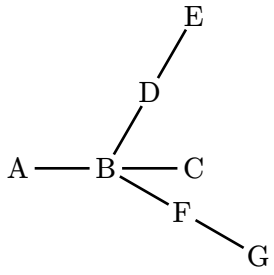
It is of course possible to have nested branches or branches with the same starting point.

```
#skeletize({
  fragment("A")
  branch({
    single(angle:1)
    fragment("B")
    branch({
      single(angle:1)
      fragment("W")
      single()
      fragment("X")
    })
    single()
    fragment("C")
  })
  branch({
    single(angle:-2)
    fragment("Y")
    single(angle:-1)
    fragment("Z")
  })
  single()
  fragment("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.

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

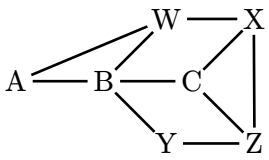


II.4 Link distant atoms

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.

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

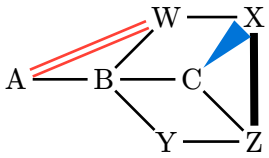


In this example, we can see that the molecules are linked to the molecules defined before with the `name` argument. Note that you can't link to a molecule that is defined after the current one because the name is not defined yet. It's a limitation of the current implementation.

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.

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



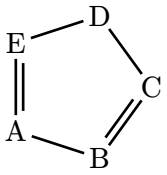
II.5 Cycles

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.

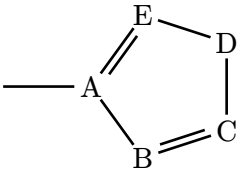
The default behavior if the angle is 0 deg is to be placed in a way that the last link is vertical.

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



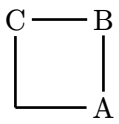
If the angle is not 0 deg or if the `align` argument is set, the cycle will be drawn in relation with the relative angle of the last link.

```
#skeletize({
  single()
  fragment("A")
  cycle(5, align: true, {
    single()
    fragment("B")
    double()
    fragment("C")
    single()
    fragment("D")
    single()
    fragment("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.

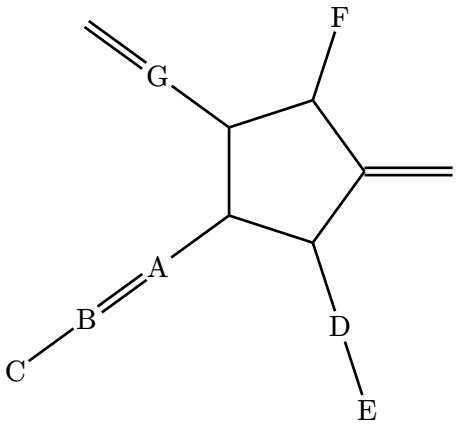
```
#skeletize({
  cycle(4,{
    single()
    fragment("A")
    single()
    fragment("B")
    single()
    fragment("C")
    single()
    fragment("D")
  })
})
```



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.

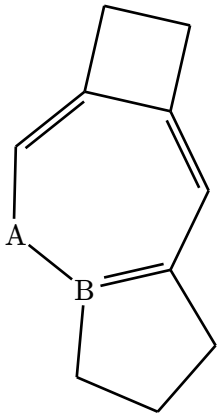
```
#skeletize({
  cycle(5,{
    branch({
      single()
      fragment("A")
      double()
      fragment("B")
      single()
      fragment("C")
    })
    single()
    branch({
      single()
      fragment("D")
      single()
      fragment("E")
    })
    single()
    branch({
      double()
    })
    single()
    branch({
      single()
      fragment("F")
    })
    single()
    branch({
      single()
      fragment("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.

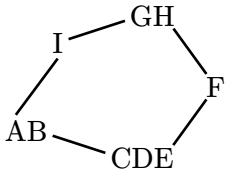
```
#skeletize({
  fragment("A")
  cycle(7,{
    single()
    fragment("B")
    cycle(5,{
      single()
      single()
      single()
      single()
    })
    double()
    single()
    double()
    cycle(4,{
      single()
      single()
      single()
    })
    single()
    double()
    single()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



II.5.4 Issues with atom groups

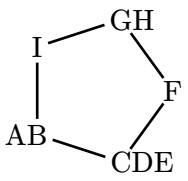
Cycles by default have an issue with atom groups with multiples atoms. The links are not well placed for the cycle to be drawn correctly.

```
#skeletize({
  fragment("AB")
  cycle(5,{
    single()
    fragment("CDE")
    single()
    fragment("F")
    single()
    fragment("GH")
    single()
    fragment("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.

```
#skeletize({
  fragment("AB")
  cycle(5,{
    single(from: 1, to: 0)
    fragment("CDE")
    single(from: 0)
    fragment("F")
    single(to: 0)
    fragment("GH")
    single(from: 0)
    fragment("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.

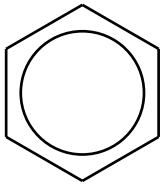
Argument

`⟨radius⟩: none` `float`

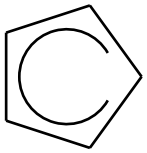
Radius of the arc in percentage of the smallest distance between two opposite atoms in the cycle. By default, it is set to 0.7 for cycle with more than 4 faces and 0.5 for cycle with 4 or 3 faces.

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

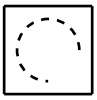
```
  #skeletize({
    cycle(6, arc:(:), {
      single()
      single()
      single()
      single()
      single()
      single()
    })
  })
```



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



```
  #skeletize({
    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:

```
1 #let single = build-link((length, ctx, _, args) => {
2   import cetz.draw: *
```

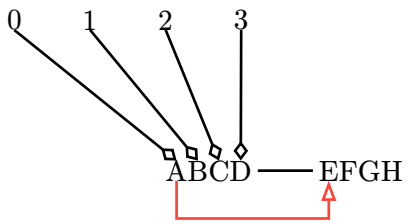
```
    line((0, 0), (length, 0), stroke: args.at("stroke", default:
    ctx.config.single.stroke))
})
```

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.

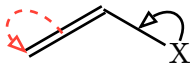
```
#skeletize({
  import cetz.draw: *
  fragment("ABCD", name: "A")
  single()
  fragment("EFGH", name: "B")
  line(
    "A.0.south",
    (rel: (0, -0.5)),
    (to: "B.0.south", rel: (0, -0.5)),
    "B.0.south",
    stroke: red,
    mark: (end: ">"),
  )
  for i in range(0, 4) {
    content((-2 + i,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



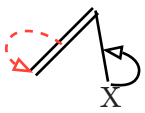
II.7.2 Links

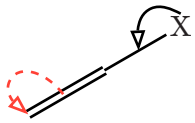
If you name your links with the `name` argument, you can use them in cetz code. The name of the link is the name of the cetz object. It exposes the same anchors as the `line` function of cetz.

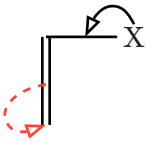
```
#skeletize({
  import cetz.draw: *
  double(absolute: 30deg, name: "l1")
  single(absolute: -30deg, name: "l2")
  fragment("X", name: "X")
  hobby(
    "l1.50%",
    ("l1.start", 0.5, 90deg, "l1.end"),
    "l1.start",
    stroke: (paint: red, dash: "dashed"),
    mark: (end: ">"),
  )
  hobby(
    (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.



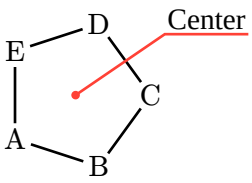




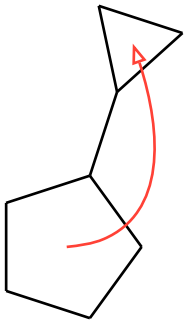
II.7.3 Cycles centers

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.

```
#skeletize({
  import cetz.draw: *
  fragment("A")
  cycle(
    5,
    name: "cycle",
    {
      single()
      fragment("B")
      single()
      fragment("C")
      single()
      fragment("D")
      single()
      fragment("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,
  )
})
```



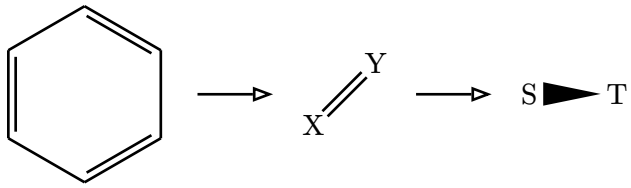
```
#skeletize({
  import cetz.draw: *
  cycle(5, name: "c1", {
    single()
    single()
    single()
    branch({
      single()
      cycle(3, name: "c2", {
        single()
        single()
        single()
      })
    })
    single()
    single()
  })
  hobby(
    "c1",
    ("c1", 0.5, -60deg, "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", {
      fragment("X")
      double(angle: 1)
      fragment("Y")
    })
  line((to: "mol2.east", rel: (1em, 0)), (rel: (1, 0)), mark: (end: ">"))
  set-origin((rel: (1em, 0)))
  draw-skeleton(name: "mol3", {
    fragment("S")
    cram-filled-right()
    fragment("T")
  })
})
```

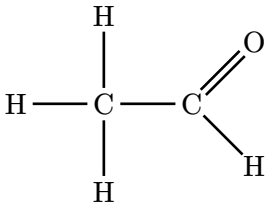


II.8 Examples

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.

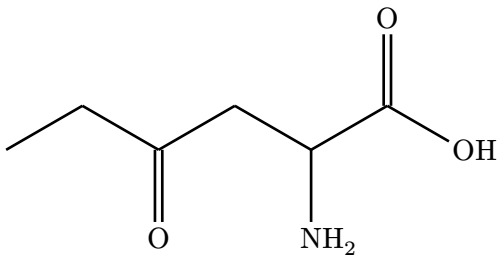
II.8.1 Ethanol

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



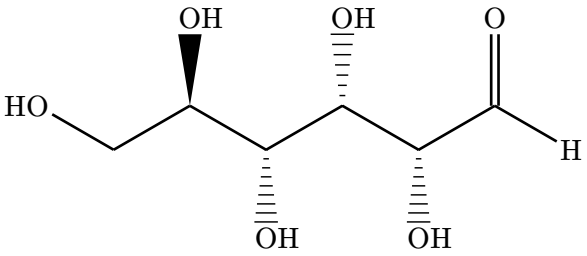
II.8.2 2-Amino-4-oxohexanoic acid

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



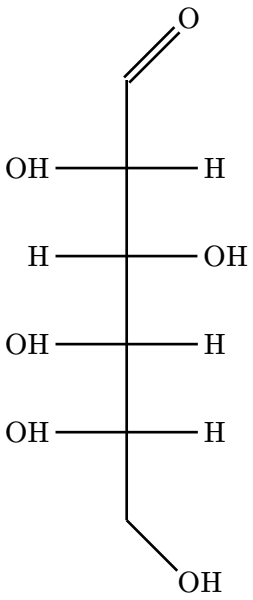
II.8.3 Glucose

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



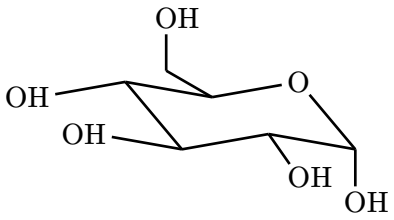
II.8.4 Fisher projection

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



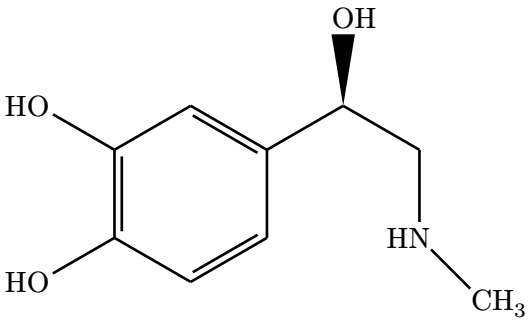
II.8.5 α-D-glucose

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



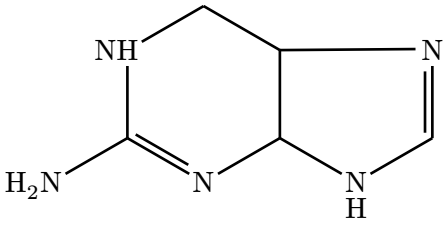
II.8.6 Adrenaline

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



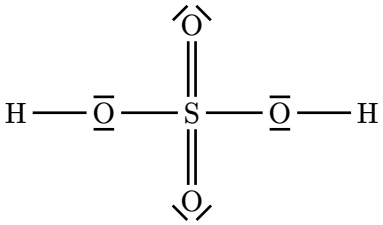
II.8.7 Guanine

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



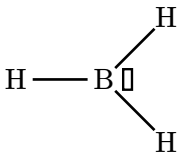
II.8.8 Sulfuric Acid

```
#skeletize({
  fragment("H")
  single()
  fragment("O", lewis: (
    lewis-line(angle: 90deg),
    lewis-line(angle: -90deg)
  ))
  single()
  fragment("S")
  let do(sign) = {
    double()
    fragment("O", lewis: (
      lewis-line(angle: sign * 45deg),
      lewis-line(angle: sign * 135deg)
    ))
  }
  branch(angle: 2, do(1))
  branch(angle: -2, do(-1))
  single()
  fragment("O", lewis: (
    lewis-line(angle: 90deg),
    lewis-line(angle: -90deg)
  ))
  single()
  fragment("H")
})
```



II.8.9 BH_3

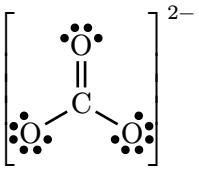
```
#skeletize({
  fragment("H")
  single()
  fragment("B", lewis: (
     lewis-rectangle(fragment-margin:
5pt),
  ))
  branch(angle:1, {
    single()
    fragment("H")
  })
  branch(angle:-1, {
    single()
    fragment("H")
  })
})
```



II.8.10 Carbonate ion

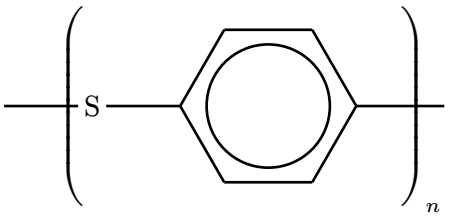
```
#skeletize(
  config: (
    atom-sep: 2em,
  ),
  {
    parenthesis(
      l: "[",
      r: "]",
      tr: $2-$,
      xoffset: .05,
      {
        fragment(
          "O",
          lewis: (
            lewis-double(angle: 135),
            lewis-double(angle: -45),
           lewis-double(angle: -135),
          ),
        )

        single(relative: 30deg)
        fragment("C")
        branch(
          angle: 2,
          {
            double()
            fragment(
              "O",
              lewis: (
               lewis-double(angle: 45),
              lewis-double(angle: 135),
              ),
            )
          },
        )
        single(absolute: -30deg)
        fragment(
          "O",
          lewis: (
            lewis-double(angle: 45),
            lewis-double(angle: -45),
           lewis-double(angle: -135),
          ),
        )
      },
    )
  },
)
```



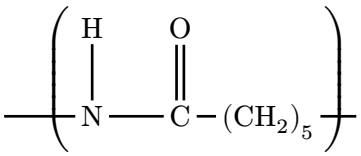
II.8.11 Polphenyl sulfide

```
#skeletize({
  single()
  parenthesis(
    br: $n$,
    right: "end",
    {
      fragment("S")
      single()
      cycle(
        6,
        align: true,
        arc: (:),
        {
          for i in range(3) {
            single()
          }
          branch(single(name: "end"))
          for i in range(3) {
            single()
          }
        },
      )
    },
  )
})
```



II.8.12 Nylon 6

```
#skeletize({
  parenthesis(xoffset: (.4, -.15), {
    single()
    fragment("N")
    branch(angle: 2, {
      single()
      fragment("H")
    })
    single()
    fragment("C")
    branch(angle: 2, {
      double()
      fragment("O")
    })
    single()
    fragment($(C H_2)_5$)
    single()
  })
})
```



Part III

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