MODIAGRAM

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Easy Creation of Molecular Orbital Diagrams

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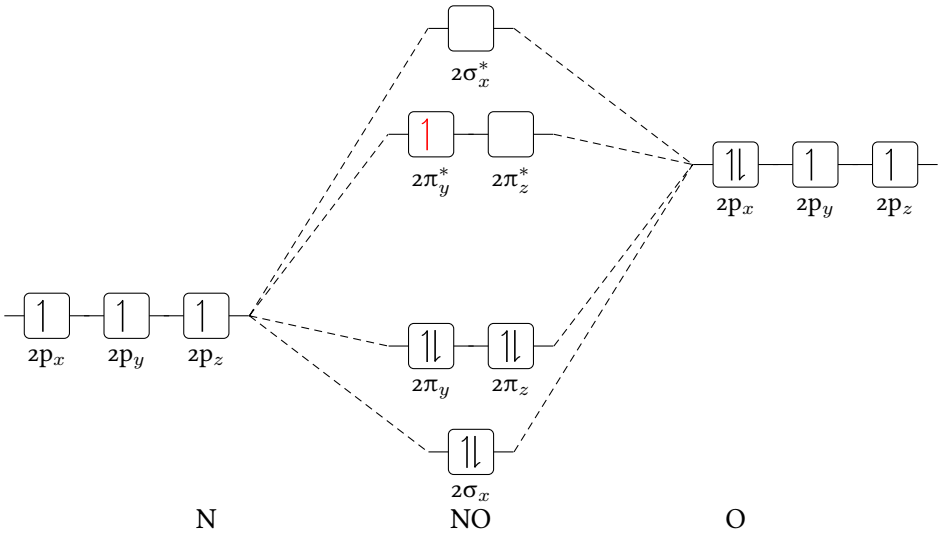
English documentation



Contents

1 Licence, Requirements

Permission is granted to copy, distribute and/or modify this software under the terms of the LaTeX Project Public License, version 1.3 or later (`http://www.latex-project.org/lppl.txt`). This package has the status "maintained."

MODIAGRAM needs and loads the packages expl3,[1] xparse,[2] l3keys2e,[3] Ti*k*Z[4] and textgreek.[5] Additionally the Ti*k*Z libraries calc and arrows are loaded. Knowledge of pgf or Ti*k*Z are helpful.

2 Motivation

This package has been written as a reaction to a question on `http://tex.stackexchange.com/`. To be more precise: as a reaction to the question "Molecular orbital diagrams in LaTeX." There it says

> I'm wondering if anyone has seen a package for drawing (qualitative) molecular orbital splitting diagrams in LaTeX? Or if there exist any packages that can be easily re-purposed to this task?
>
> Otherwise, I think I'll have a go at it in Ti*k*Z.

The problem was solved using Ti*k*Z, since no package existed for that purpose. For one thing MODIAGRAM is intended to fill this gap. I also found it very tedious, to make all this copying and pasting when I needed a second, third, ... diagram. MODIAGRAM took care of that.

3 Main Commands

All molecular orbital (MO) diagrams are created using the environment `\begin{MOdiagram}` `\end{MOdiagram}`.

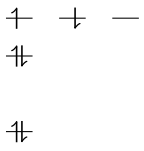
[1] CTAN: expl3 [2] CTAN: xparse [3] CTAN: l3keys2e [4] CTAN: Ti*k*Z [5] CTAN: textgreek

3.1 The \atom Command

▸ `\atom[<name>]{left|right}{<AO-spec>}`
`[<name>]` caption of the atom;
`{left|right}` on the left or the right in the diagram;
`{<AO-spec>}` specifications of the atomic orbitals (AOs).

Let's take a look at an example:

```
\begin{MOdiagram}
 \atom{right}{
   1s = {  0; pair} ,
   2s = {  1; pair} ,
   2p = {1.5; up, down }
 }
\end{MOdiagram}
```



As you can see, the argument `{<AO-spec>}` is essential to create the actual orbitals and the electrons within. You can use these key/value pairs to specify what you need:

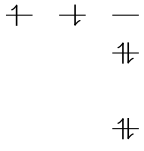
▸ `1s = <rel-energy>; <el-spec>`

▸ `2s = <rel-energy>; <el-spec>`

▸ `2p = <rel-energy>; <x el-spec>, <y el-spec>, <z el-spec>`
`<el-spec>` can have the values `pair`, `up` and `down` or can be left empty. `<rel-energy>` actually is the y coordinate and shifts the AO vertically by `<rel-energy>` cm.

The argument `{left|right}` is important, when p orbitals are used. For instance compare the following example to the one before:

```
\begin{MOdiagram}
 \atom{left}{
   1s = {  0; pair} ,
   2s = {  1; pair} ,
   2p = {1.5; up, down }
 }
\end{MOdiagram}
```



When both variants are used one can also see, that the right atom is shifted to the right (hence the naming). The right atom is shifted by 4 cm per default and can be adjusted individually, see page 17.

```
\begin{MOdiagram}
 \atom{left}{
   1s = {  0; pair} ,
   2s = {  1; pair} ,
   2p = {1.5; up, down }
 }
 \atom{right}{
   1s = {  0; pair} ,
   2s = {  1; pair} ,
   2p = {1.5; up, down }
 }
\end{MOdiagram}
```

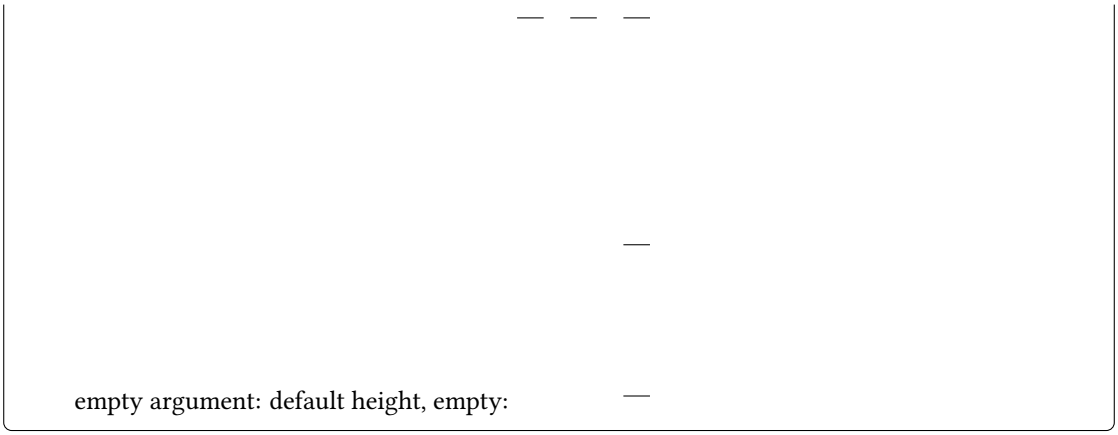
With the command \molecule (section 3.2) the reason for the shift becomes clear.

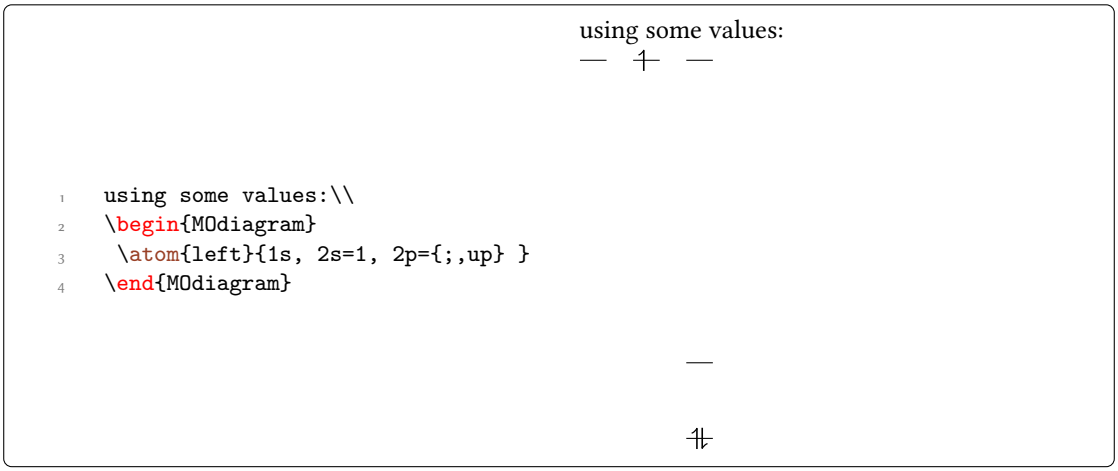
Any of the arguments for the AO can be left empty or be omitted.

```
Without argument: default height, full:
\begin{MOdiagram}
 \atom{left}{1s, 2s, 2p}
\end{MOdiagram}
```

Without argument: default height, full:

```
empty argument: default height, empty:
\begin{MOdiagram}
 \atom{left}{1s=, 2s=, 2p=}
\end{MOdiagram}
```

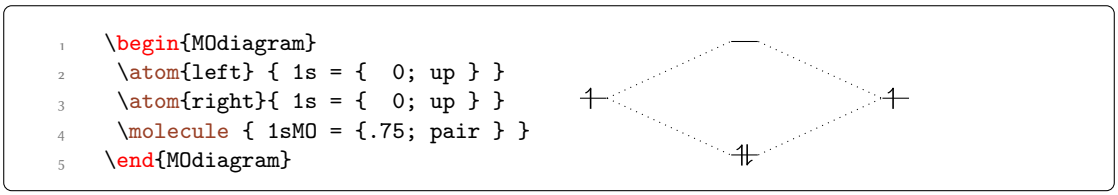




3.2 The \molecule Command

▸ \molecule[<name>]{<MO-spec>}
[<name>] caption of the molecule;
{<MO-spec>} specifications of the molecular orbitals (MOs);

An example first:



The command \molecule connects the AOs with the bonding and anti-bondung MOs. \molecule can only be used *after* one has set *both* atoms since the orbitals that are to be connected must be known.

The argument {<MO-spec>} accepts a comma separated list of key/value pairs:

- `1sMO = <energy gain>/<energy loss>; <s el-spec>, <s* el-spec>` → connects the AOs specified by `1s`.
- `2sMO = <energy gain>/<energy loss>; <s el-spec>, <s* el-spec>` → connects the AOs specified by `2s`.
- `2pMO = <s energy gain>/<s energy loss>, <p energy gain>/<p energy loss>; <s el-spec>, <py el-spec>, <pz el- spec>, <py* el-spec>, <pz* el-spec>, <s* el-spec>` → connects the AOs specified by `2p`.

  Obviously the regarding AOs must have been set in order to connect them. This for example won't work:

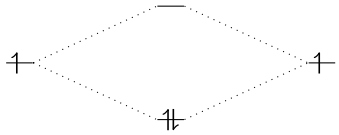
```
\begin{MOdiagram}
 \atom{left} { 1s = 0 }
 \atom{right}{ 1s = 0 }
 \molecule { 2sMO = .75 }
\end{MOdiagram}
```

  The value used in `<energy gain>` determines how many cm the bonding MO lies below the lower AO or how many cm the anti-bondung MO lies above the higher AO.

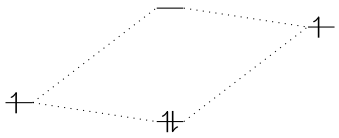
```
same level:
\begin{MOdiagram}
 \atom{left} { 1s = {  0; up } }
 \atom{right}{ 1s = {  0; up } }
 \molecule { 1sMO = {.75; pair } }
\end{MOdiagram}

different levels:
\begin{MOdiagram}
 \atom{left} { 1s = {  0; up } }
 \atom{right}{ 1s = {  1; up } }
 \molecule { 1sMO = {.25; pair } }
\end{MOdiagram}
```

same level:



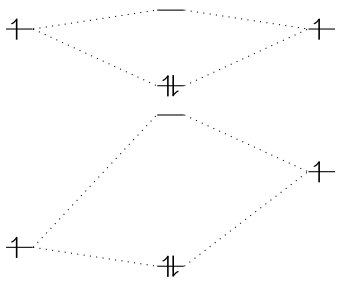
different levels:



  If you specify `<energy loss>` you can create non-symmetrical splittings. Then, the first value (`<energy gain>`) is used for the bonding MO and the second value (`<energy loss>`) is used for the anti-bonding MO.

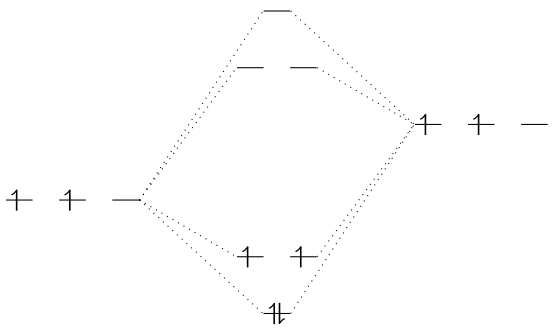
```
\begin{MOdiagram}
 \atom{left} { 1s = {  0; up } }
 \atom{right}{ 1s = {  0; up } }
 \molecule { 1sMO = {.75/.25; pair } }
\end{MOdiagram}

\begin{MOdiagram}
 \atom{left} { 1s = {  0; up } }
 \atom{right}{ 1s = {  1; up } }
 \molecule { 1sMO = {.25/.75; pair } }
\end{MOdiagram}
```



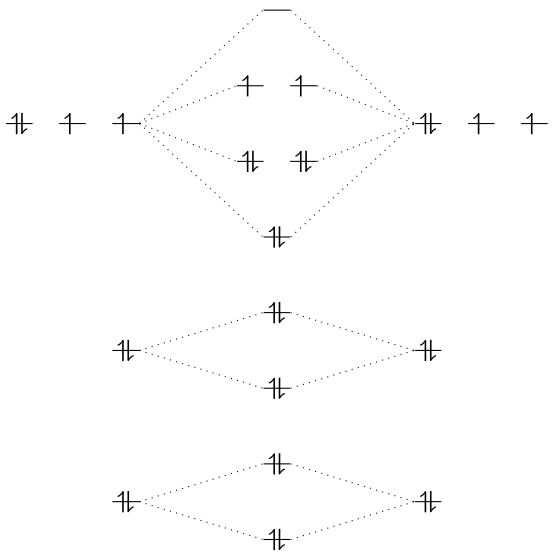
Please be aware, that you have to specify *two* such values or pairs with `2pMO`: the splitting of the σ orbitals and the splitting of the π orbitals.

```
\begin{MOdiagram}
 \atom{left} { 2p = { 0; up, up } }
 \atom{right}{ 2p = { 1; up, up } }
 \molecule { 2pMO = { 1.5, .75; pair, up, up } }
\end{MOdiagram}
```



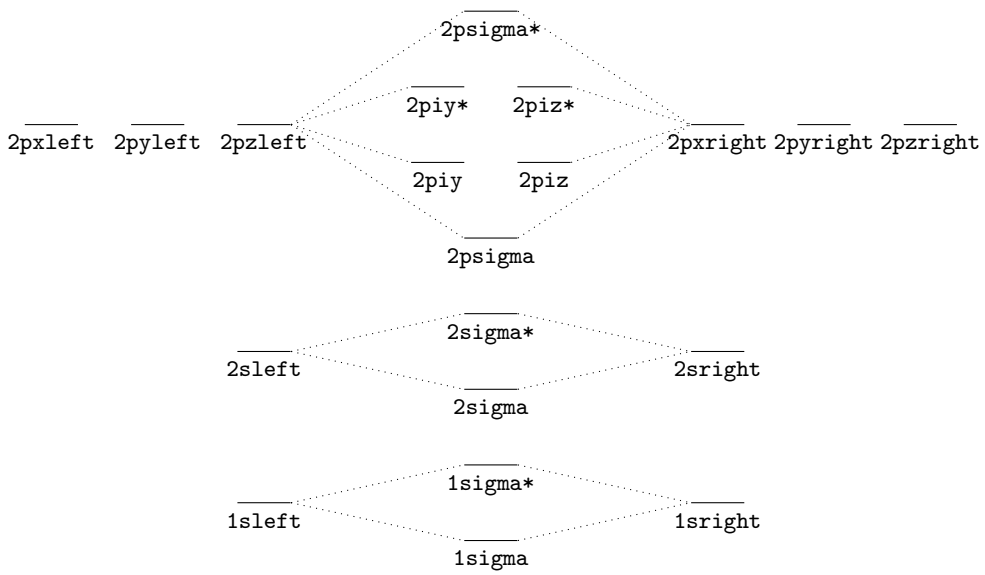
The complete MO diagram for triplett dioxygen now could look something like that:

```
\begin{MOdiagram}
 \atom{left}{
   1s, 2s, 2p = {;pair,up,up}
 }
 \atom{right}{
   1s, 2s, 2p = {;pair,up,up}
 }
 \molecule{
   1sMO, 2sMO, 2pMO = {;pair,pair,pair,up,up}
 }
\end{MOdiagram}
```



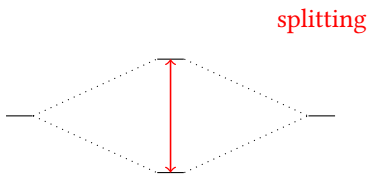
3.3 The Naming Scheme

Since one wants to be able to put labels to the orbitals and since they are nodes in a `tikzpicture`, the internal naming scheme is important. It closely follows the function:

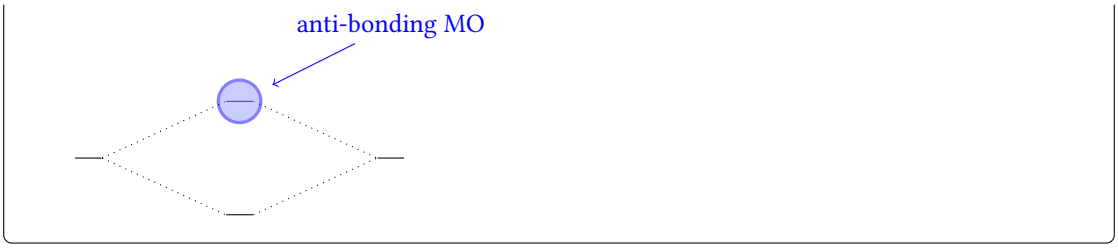


With these names it is possible to reference the orbitals with the known Ti*k*Z commands:

```
\begin{MOdiagram}
 \atom{left} { 1s = 0 }
 \atom{right}{ 1s = 0 }
 \molecule { 1sMO = .75 }
 \draw[<->,red,semithick] (1sigma.center) -- (1sigma*.center) ;
 \draw[red] (1sigma*) ++ (2cm,.5cm) node {splitting} ;
\end{MOdiagram}
```

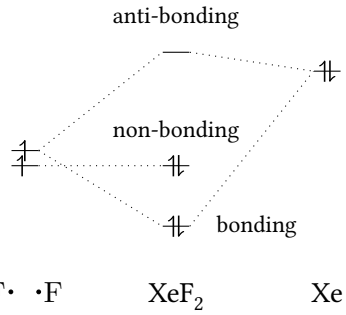



```
\begin{MOdiagram}
 \atom{left} { 1s = 0 }
 \atom{right}{ 1s = 0 }
 \molecule { 1sMO = .75 }
 \draw[draw=blue,very thick,fill=blue!40,opacity=.5] (1sigma*) circle
  (8pt);
 \draw[<-,shorten <=8pt,shorten >=15pt,blue] (1sigma*) --++(2,1) node
  {anti-bonding MO};
\end{MOdiagram}
```



3.4 Placing AOs and MOs Arbitrarily

The standard orbitals are not always sufficient in order to draw a correct MO diagram. For example in the MO diagram of XeF_2 one would need the part that illustrates the interaction between the bonding and anti-bonding combination of two p orbitals of Flourine with one p orbital of Xenon:

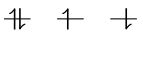


To create diagrams like this there is the following command, which draws a single AO:

▸ `\AO[<name>](<xshift>){<type>}[<key = val>]{<energy>;<el-spec>}`
`[<name>]` (optional) name of the node; if not specified, `AO#` is used where `#` is a consecutive number.
`[<xshift>]` vertical position of the orbitals, a TEX dimension.
`{<type>}` `s` or `p`.
`[<key = val>]` key/value pairs with which the AO can be customized, see section 4.3.
`{<AO-spec>}` specification of the AO.

Depending on the `<type>` one s or three p orbitals are drawn.

```
\begin{MOdiagram}
 \AO{s}{0;}
 \AO(-20pt){p}{1;pair,up,down}
\end{MOdiagram}
```

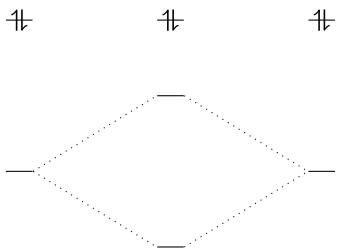


If one wants to place such an AO at the position of an atom, one has to know their `<xshift>`. They have predefined values (also see section 3.5):

- atom left: 1 cm

- molecule: 3 cm
- atom right: 5 cm

```
\begin{MOdiagram}
 \atom{left} {1s=0}
 \atom{right}{1s=0}
 \molecule {1sMO=1}
 \AO(1cm){s}{2}
 \AO(3cm){s}{2}
 \AO(5cm){s}{2}
\end{MOdiagram}
```

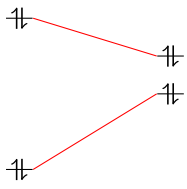


Within the p orbitals there is an additional shift by 20 pt per orbital. This is equivalent to a double shift by the length `AO-width` (see section 4.1.3):

```
\begin{MOdiagram}
 \atom{left} {2p=0}
 \atom{right}{2p=0}
 % above the left atom:
 \AO(1cm)     {s}{ .5}
 \AO(1cm-20pt){s}{  1;up}
 \AO(1cm-40pt){s}{1,5;down}
 % above the right atom:
 \AO(5cm)     {s}{ .5}
 \AO(5cm+20pt){s}{  1;up}
 \AO(5cm+40pt){s}{1.5;down}
\end{MOdiagram}
```

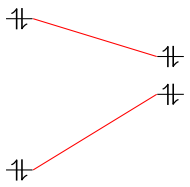
The AOs created with `\AO` also can be connected. For this you can use the Ti*k*Z command `\draw`, of course. You can use the predefined node names…

```
\begin{MOdiagram}
 \AO{s}{0} \AO(2cm){s}{1}
 \AO{s}{2} \AO(2cm){s}{1.5}
 \draw[red] (AO1.0) -- (AO2.180) (AO3.0) -- (AO4.180);
\end{MOdiagram}
```



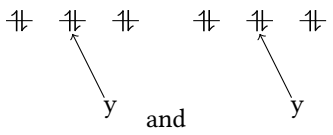
… or use own node names

```
\begin{MOdiagram}
 \AO[a]{s}{0} \AO[b](2cm){s}{1}
 \AO[c]{s}{2} \AO[d](2cm){s}{1.5}
 \draw[red] (a.0) -- (b.180) (c.0) -- (d.180);
\end{MOdiagram}
```



The predefined names are `AO1`, `AO2` etc. for the type `s` and `AO1x`, `AO1y`, `AO1z`, `AO2x` etc. for the type `p`. Nodes of the type `p` get an `x`, `y` or `z` if you specify your own name, too.

```
\begin{MOdiagram}
 \AO{p}{0}
 \draw[<-,shorten >=5pt] (AO1y.-90) -- ++ (.5,-1) node {y};
\end{MOdiagram}
and
\begin{MOdiagram}
 \AO[A]{p}{0}
 \draw[<-,shorten >=5pt] (Ay.-90) -- ++ (.5,-1) node {y};
\end{MOdiagram}
```

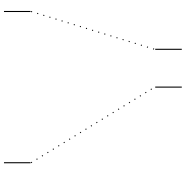


However, if you want the lines to be drawn in the same style as the ones created by `\molecule`,[6] you should use the command `\connect`.

▸ `\connect{<AO-connect>}`
`{<AO-connect>}` comma separated list of node name pairs connected with `&`.

This command expects a comma separated list of node name pairs that are to be connected. The names have to be connected with a `&`:

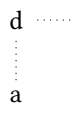
```
\begin{MOdiagram}
 \AO{s}{0;} \AO(2cm){s}{1;}
 \AO{s}{2;} \AO(2cm){s}{1.5;}
 \connect{ AO1 & AO2, AO3 & AO4 }
\end{MOdiagram}
```



[6] which can be customized, see page 20

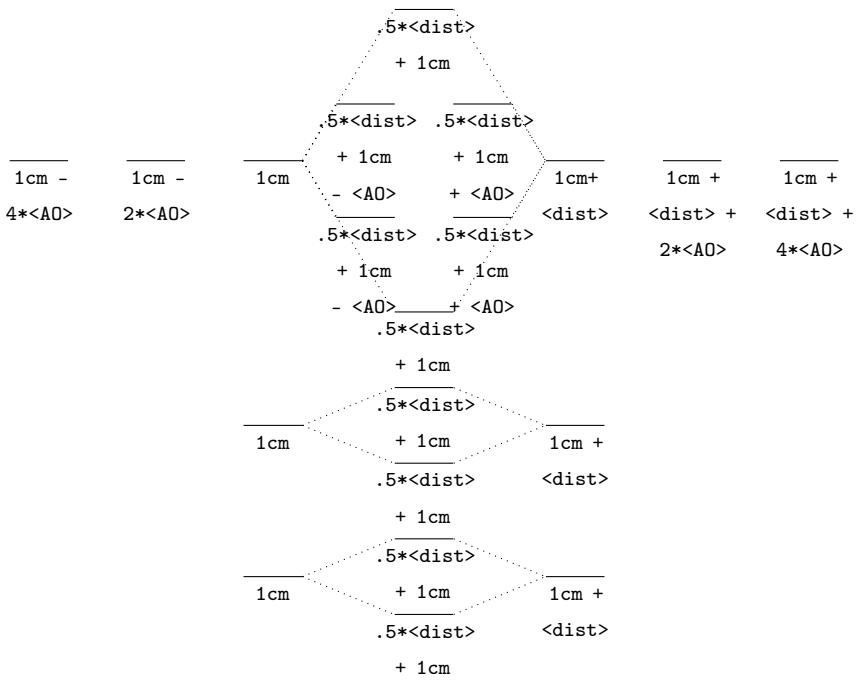
Some things still need to be said: `\connect` adds the anchor `east` to the first name and the anchor `west` to the second one. This means a connection only makes sense from the left to the right. However, you can add own anchors using the usual Ti*k*Z way:

```
\begin{tikzpicture}
 \draw (0,0) node (a) {a} ++ (1,0) node (b) {b}
       ++ (0,1) node (c) {c} ++ (-1,0) node (d) {d} ;
 \connect{ a.90 & d.-90, c.180 & d.0 }
\end{tikzpicture}
```



3.5 The Positioning Scheme

The figure below shows the values of the x coordinates of the orbitals depending on the values of `<distance>` (`<dist>`) and `<AO-width>` (`<AO>`). In sections 4.1.2 and 4.1.3 these lengths and how they can be changed are discussed.



3.6 Default Values

If you leave the arguments (or better: values) for the specification of the AO or MO empty or omit them, default values are used. The table below shows you, which ones.

	AO/MO	omitted	empty
syntax:		1s	1s=
	1s	{0;pair}	{0;}
	2s	{2;pair}	{2;}
	2p	{5;pair,pair,pair}	{5;,,}
	1sMO	{.5;pair,pair}	{.5;,}
	2sMO	{.5;pair,pair}	{.5;,}
	2pMO	{1.5,.5;pair,pair,pair,pair,pair,pair}	{1.5,.5;,,,,,}

This is similar for the \AO command (page 10); it needs a value for <energy>, though.

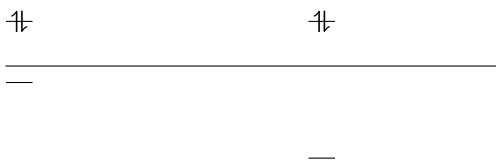
<type>	<el-spec>
s	pair
p	pair,pair,pair

Compare these examples:

```
\begin{MOdiagram}
 \atom{left} { 1s={0;pair} }
 \atom{right}{ 1s }
\end{MOdiagram}

\hrulefill

\begin{MOdiagram}
 \atom{left}{ 1s=1 }
 \atom{right}{ 1s= }
\end{MOdiagram}
```



4 Customization

Th options of the section 4.1 can be set global as package option, i.e. with \usepackage[<key = val>]{modiagram}, or via the setup command \MOsetup{<key = val>}.

4.1 Environment Options

There are some options with which the layout of the MO diagrams can be changed:

- style = <type> ⟶ change the style of the orbitals and the connecting lines, section 4.1.1.
- distance = <dim> ⟶ distance betwen left and right atom, section 4.1.2.
- AO-width = <dim> ⟶ change the width of orbitals, section 4.1.3.
- el-sep = <num> ⟶ distance between the electron pair arrows, section 4.1.4.
- up-el-pos = <num> ⟶ position of the spin-up arrow, section 4.1.4.

- down-el-pos = <num> ⟶ position of the spin-down arrow, section 4.1.4.
- lines = <tikz> ⟶ change the Ti*k*Z style of the connecting lines, section 4.1.5.
- names = <bool> ⟶ add captions to the atoms and the molecule, section 4.1.6.
- names-style = <tikz> ⟶ change the Ti*k*Z style of the captions, section 4.1.7.
- names-style-add = <tikz> ⟶ change the Ti*k*Z style of the captions, section 4.1.7.
- labels = <bool> ⟶ add default labels to the orbitals, section 4.1.8.
- labels-fs = <cs> ⟶ change the font size of the labels, section 4.1.9.
- labels-style = <tikz> ⟶ change the Ti*k*Z style of the labels, section 4.1.10.

They all are discussed in the following sections. If they're used as options for the environment, they'r set locally and only change that environment.

```
\begin{MOdiagram}[<key = value>]
 ...
\end{MOdiagram}
```

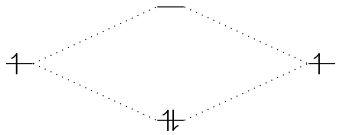
4.1.1 Option style

There are five different styles which can be chosen.

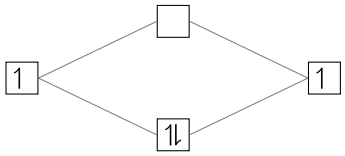
- style = plain ⇅ (default)
- style = square ⇅
- style = circle ⇅
- style = round ⇅
- style = fancy ⇅

Let's take the MO diagram of H_2 to illustrate the different styles:

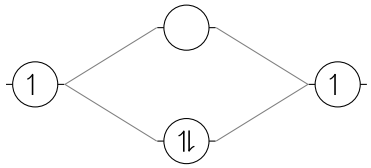
```
% use package 'chemmacros'
\begin{MOdiagram}[style=plain]% default
 \atom[H]{left} { 1s = {;up} }
 \atom[H]{right}{ 1s = {;up} }
 \molecule[\ch{H2}]{ 1sMO = {.75;pair} }
\end{MOdiagram}
```



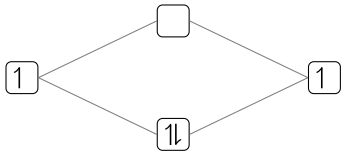
```
% use package ‘chemmacros’
\begin{MOdiagram}[style=square]
 \atom[H]{left} { 1s = {;up} }
 \atom[H]{right}{ 1s = {;up} }
 \molecule[\ch{H2}]{ 1sMO = {.75;pair} }
\end{MOdiagram}
```



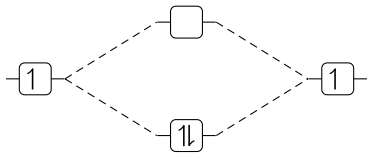
```
% use package ‘chemmacros’
\begin{MOdiagram}[style=circle]
 \atom[H]{left} { 1s = {;up} }
 \atom[H]{right}{ 1s = {;up} }
 \molecule[\ch{H2}]{ 1sMO = {.75;pair} }
\end{MOdiagram}
```



```
% use package ‘chemmacros’
\begin{MOdiagram}[style=round]
 \atom[H]{left} { 1s = {;up} }
 \atom[H]{right}{ 1s = {;up} }
 \molecule[\ch{H2}]{ 1sMO = {.75;pair} }
\end{MOdiagram}
```



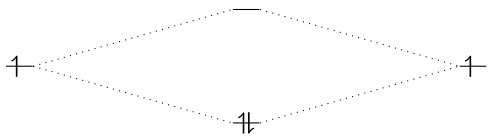
```
% use package 'chemmacros'
\begin{MOdiagram}[style=fancy]
 \atom[H]{left} { 1s = {;up} }
 \atom[H]{right}{ 1s = {;up} }
 \molecule[\ch{H2}]{ 1sMO = {.75;pair} }
\end{MOdiagram}
```



4.1.2 Option `distance`

Depending on labels and captions the 4 cm by which the right and left atom are separated can be too small. With `distance = <dim>` the length can be adjusted. This will change the position of the right atom to `1cm + <dim>` and the position of the molecule is changed to `0.5*(1cm + <dim>)`, also see page 10 and section 3.5.

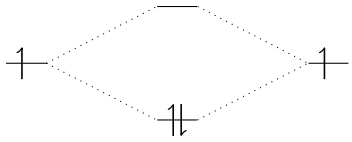
```
% use package 'chemmacros'
\begin{MOdiagram}[distance=6cm]
 \atom[H]{left} { 1s = {;up} }
 \atom[H]{right}{ 1s = {;up} }
 \molecule[\ch{H2}]{ 1sMO = {.75;pair} }
\end{MOdiagram}
```



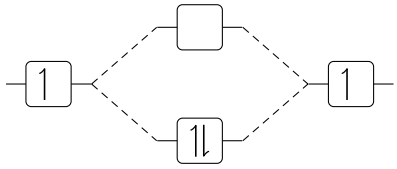
4.1.3 Option `AO-width`

The length `AO-width` sets the length of the horizontal line in a orbital displayed with the `plain` style. It's default value is 10 pt.

```
% use package 'chemmacros'
\begin{MOdiagram}[AO-width=15pt]
 \atom[H]{left} { 1s = {;up} }
 \atom[H]{right}{ 1s = {;up} }
 \molecule[\ch{H2}]{ 1sMO = {.75;pair} }
\end{MOdiagram}
```



```
% use package 'chemmacros'
\begin{MOdiagram}[style=fancy,AO-width=15pt]
 \atom[H]{left} { 1s = {;up} }
 \atom[H]{right}{ 1s = {;up} }
 \molecule[\ch{H2}]{ 1sMO = {.75;pair} }
\end{MOdiagram}
```

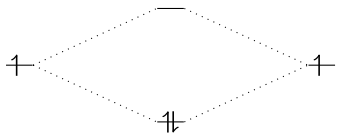


By changing the value of `AO-width` the positions of the p and the π orbitals also change, see section 3.5.

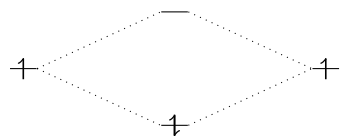
4.1.4 Optionen `el-sep`, `up-el-pos` und `down-el-pos`

These three options change the horizontal positions of the arrows representing the electrons in an AO/MO. The option `el-sep = <num>` needs a value between 0 and 1. 0 means *no* distance between the arrows and 1 *full* distance (with respect to the length `AO-width`, see section 4.1.3).

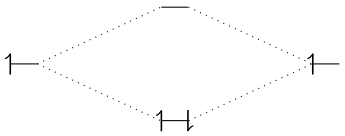
```
% use package 'chemmacros'
\begin{MOdiagram}[el-sep=.2]% default
 \atom[H]{left} { 1s = {;up} }
 \atom[H]{right}{ 1s = {;up} }
 \molecule[\ch{H2}]{ 1sMO = {.75;pair} }
\end{MOdiagram}
```



```
% use package 'chemmacros'
\begin{MOdiagram}[el-sep=0]
 \atom[H]{left} { 1s = {;up} }
 \atom[H]{right}{ 1s = {;up} }
 \molecule[\ch{H2}]{ 1sMO = {.75;pair} }
\end{MOdiagram}
```

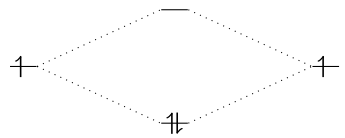


```
% use package ‘chemmacros’
\begin{MOdiagram}[el-sep=1]
 \atom[H]{left} { 1s = {;up} }
 \atom[H]{right}{ 1s = {;up} }
 \molecule[\ch{H2}]{ 1sMO = {.75;pair} }
\end{MOdiagram}
```

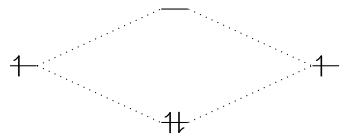


The options `up-el-pos = <num>` and `down-el-pos = <num>` can be used alternatively to place the spin-up and spin-down electron, respectively. Again they need values between 0 and 1. This time 0 means *on the left* and 1 means *on the right*.

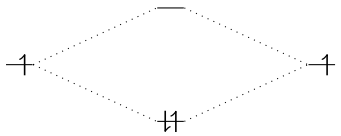
```
% use package ‘chemmacros’
\begin{MOdiagram}[up-el-pos=.4,down-el-pos=.6]% default
 \atom[H]{left} { 1s = {;up} }
 \atom[H]{right}{ 1s = {;up} }
 \molecule[\ch{H2}]{ 1sMO = {.75;pair} }
\end{MOdiagram}
```



```
% use package ‘chemmacros’
\begin{MOdiagram}[up-el-pos=.333,down-el-pos=.667]
 \atom[H]{left} { 1s = {;up} }
 \atom[H]{right}{ 1s = {;up} }
 \molecule[\ch{H2}]{ 1sMO = {.75;pair} }
\end{MOdiagram}
```



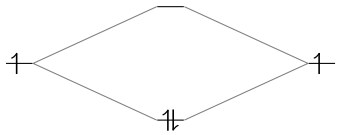
```
% use package 'chemmacros'
\begin{MOdiagram}[up-el-pos=.7,down-el-pos=.3]
 \atom[H]{left} { 1s = {;up} }
 \atom[H]{right}{ 1s = {;up} }
 \molecule[\ch{H2}]{ 1sMO = {.75;pair} }
\end{MOdiagram}
```



4.1.5 Option `lines`

The option `lines` can be used to modify the Ti*k*Z style of the connecting lines:

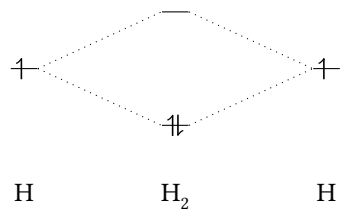
```
% use package 'chemmacros'
\begin{MOdiagram}[lines={gray,thin}]
 \atom[H]{left} { 1s = {;up} }
 \atom[H]{right}{ 1s = {;up} }
 \molecule[\ch{H2}]{ 1sMO = {.75;pair} }
\end{MOdiagram}
```



4.1.6 Option `names`

If you use the option `names` the atoms and the molecule get captions provided you have used the optional <name> argument of `\atom` and/or `\molecule`.

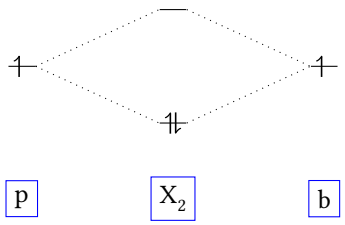
```
% use package 'chemmacros'
\begin{MOdiagram}[names]
 \atom[H]{left} { 1s = {;up} }
 \atom[H]{right}{ 1s = {;up} }
 \molecule[\ch{H2}]{ 1sMO = {.75;pair} }
\end{MOdiagram}
```



4.1.7 Optionens names-style and names-style-add

These options enable to customize the style of the captions of the atoms and of the molecule. By default this setting is used: `names-style = {anchor=base}`.[7]

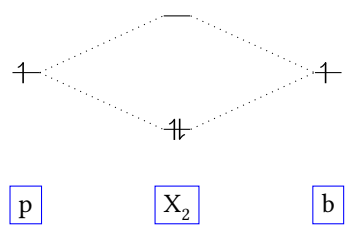
```
% use package 'chemmacros'
\begin{MOdiagram}[names,names-style={draw=blue}]
 \atom[p]{left} { 1s = {;up} }
 \atom[b]{right}{ 1s = {;up} }
 \molecule[\ch{X2}]{ 1sMO = {.75;pair} }
\end{MOdiagram}
```



With this the default setting is overwritten. As you can see it destroys the vertical alignment of the nodes. In order to avoid that you can for example specify `text height` and `text depth` yourself ...

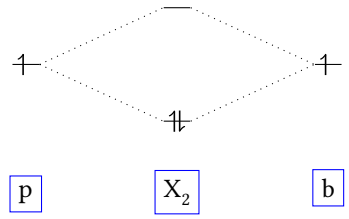
```
% use package 'chemmacros'
\begin{MOdiagram}[names,names-style={text height=1.5ex, text depth
 =.25ex, draw=blue}]
 \atom[p]{left} { 1s = {;up} }
 \atom[b]{right}{ 1s = {;up} }
 \molecule[\ch{X2}]{ 1sMO = {.75;pair} }
\end{MOdiagram}
```

[7] Please see "Ti*k*Z and PGF – Manual for Version 2.10" p. 183 section 16.4.4 (pgfmanual.pdf) for the meaning



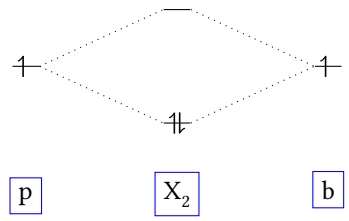
…, add the anchor again …

```
% use package ‘chemmacros’
\begin{MOdiagram}[names,names-style={anchor=base, draw=blue}]
 \atom[p]{left} { 1s = {;up} }
 \atom[b]{right}{ 1s = {;up} }
 \molecule[\ch{X2}]{ 1sMO = {.75;pair} }
\end{MOdiagram}
```

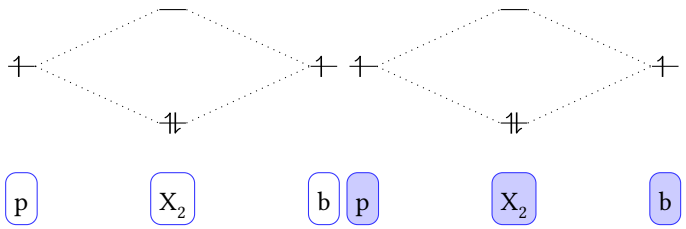


… or use the option names-style-add. It doesn’t overwrite the current setting but appends the new declaration:

```
% use package ‘chemmacros’
\begin{MOdiagram}[names,names-style-add={draw=blue}]
 \atom[p]{left} { 1s = {;up} }
 \atom[b]{right}{ 1s = {;up} }
 \molecule[\ch{X2}]{ 1sMO = {.75;pair} }
\end{MOdiagram}
```



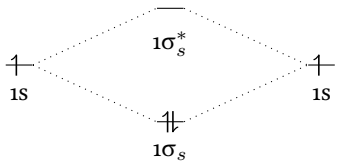
```
% use package 'chemmacros'
\MOsetup{names,names-style={text height=2.5ex,text depth=.5ex,draw=
 blue!80,rounded corners}}
\begin{MOdiagram}
 \atom[p]{left} { 1s = {;up} }
 \atom[b]{right}{ 1s = {;up} }
 \molecule[\ch{X2}]{ 1sMO = {.75;pair} }
\end{MOdiagram}
\begin{MOdiagram}[names-style-add={fill=blue!20}]
 \atom[p]{left} { 1s = {;up} }
 \atom[b]{right}{ 1s = {;up} }
 \molecule[\ch{X2}]{ 1sMO = {.75;pair} }
\end{MOdiagram}
```



4.1.8 Option labels

If you use the option labels predefined labels are written below the orbitals. These labels can be changed, see section 4.2.1.

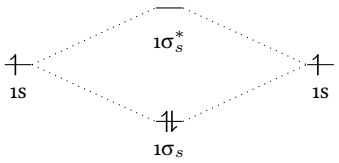
```
% use package 'chemmacros'
\begin{MOdiagram}[labels]
 \atom[H]{left} { 1s = {;up} }
 \atom[H]{right}{ 1s = {;up} }
 \molecule[\ch{H2}]{ 1sMO = {.75;pair} }
\end{MOdiagram}
```



4.1.9 Option labels-fs

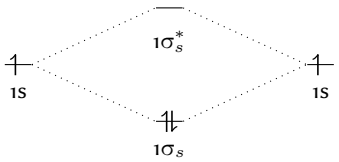
Labels are set with the font size \small. If you want to change that you can use the option labels-fs.

```
% use package 'chemmacros'
\begin{MOdiagram}[labels,labels-fs=\footnotesize]
 \atom[H]{left} { 1s = {;up} }
 \atom[H]{right}{ 1s = {;up} }
 \molecule[\ch{H2}]{ 1sMO = {.75;pair} }
\end{MOdiagram}
```



This also allows you to change the font style or font shape of the labels.

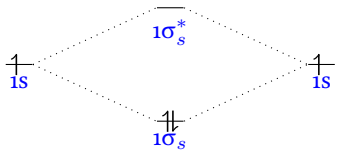
```
% use package 'chemmacros'
\begin{MOdiagram}[labels,labels-fs=\sffamily\footnotesize]
 \atom[H]{left} { 1s = {;up} }
 \atom[H]{right}{ 1s = {;up} }
 \molecule[\ch{H2}]{ 1sMO = {.75;pair} }
\end{MOdiagram}
```



4.1.10 Option `labels-style`

The option `labels-style` changes the Ti*k*Z style of the nodes within which the labels are written.

```
% use package 'chemmacros'
\begin{MOdiagram}[labels,labels-style={blue,yshift=4pt}]
 \atom[H]{left} { 1s = {;up} }
 \atom[H]{right}{ 1s = {;up} }
 \molecule[\ch{H2}]{ 1sMO = {.75;pair} }
\end{MOdiagram}
```

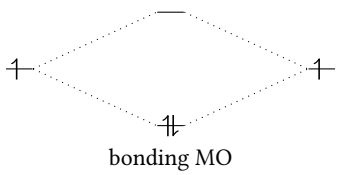


4.2 \atom and \molecule Specific Customizations

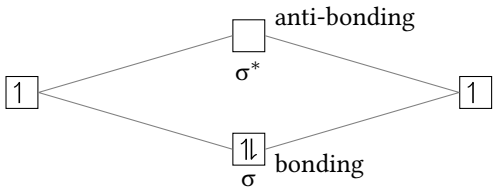
4.2.1 The label Key

If you don't want to use the predefined labels, change single labels or use only one or two labels, you can use the key label. This key is used in the \atom and \molecule commands in the <AO-spec> or <MO-spec> argument, respectively. The key awaits a comma separated key/value list. The names mentioned in section 3.3 are used as keys to specify the AO that you want to label.

```
% use package 'chemmacros'
\begin{MOdiagram}[labels-fs=\footnotesize]
 \atom[H]{left} { 1s = {;up} }
 \atom[H]{right}{ 1s = {;up} }
 \molecule[\ch{H2}]{
   1sMO  = {.75;pair},
   label = { 1sigma = {bonding MO} }
 }
\end{MOdiagram}
```

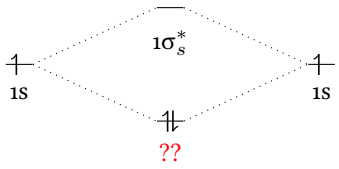



```
\begin{MOdiagram}[style=square,distance=6cm]
 \atom{left} { 1s = {;up} }
 \atom{right}{ 1s = {;up} }
 \molecule{
   1sMO  = {.75;pair} ,
   label = {
     1sigma  = \textsigma,
     1sigma* = \textsigma$^*$
   }
 }
 \node[right] at (1sigma.-45) {bonding};
 \node[right] at (1sigma*.45) {anti-bonding};
\end{MOdiagram}
```



If the key is used together with the labels option (page 23) single labels are overwritten:

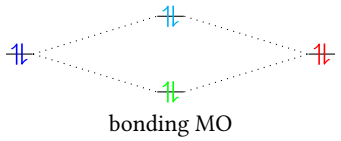
```
% use package 'chemmacros'
\begin{MOdiagram}[labels]
 \atom[H]{left} { 1s = {;up} }
 \atom[H]{right}{ 1s = {;up} }
 \molecule[\ch{H2}]{
   1sMO  = {.75;pair},
   label = { 1sigma = \textcolor{red}{??} }
 }
\end{MOdiagram}
```



4.2.2 The `color` Key

Analogous to the `label` key the `color` key can be used to display coloured electrons:

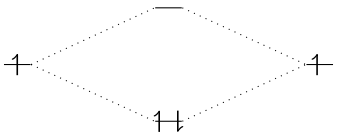
```
% use package 'chemmacros'
\begin{MOdiagram}[labels-fs=\footnotesize]
 \atom[H]{left}{
   1s, color = { 1sleft = blue }
 }
 \atom[H]{right}{
   1s, color = { 1sright = red }
 }
 \molecule[\ch{H2}]{
   1sMO,
   label = { 1sigma = {bonding MO} },
   color = { 1sigma = green, 1sigma* = cyan }
 }
\end{MOdiagram}
```



4.2.3 The `up-el-pos` and `down-el-pos` keys

The keys `up-el-pos` and `down-el-pos` allow it to shift the arrows representing the electrons in a single AO or MO individually. You need to use values between 0 and 1, also see section 4.1.4.

```
% use package 'chemmacros'
\begin{MOdiagram}
 \atom[H]{left}{
   1s        = {;up},
   up-el-pos = { 1sleft=.5 }
 }
 \atom[H]{right}{ 1s = {;up} }
 \molecule[\ch{H2}]{
   1sMO        = {.75;pair} ,
   up-el-pos   = { 1sigma=.15 } ,
   down-el-pos = { 1sigma=.85 }
 }
\end{MOdiagram}
```



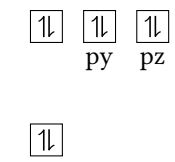
4.3 \AO Specific Customizations

These keys enable to customize orbitals created with \AO.

4.3.1 The label Key

The key label[x/y/z] allows you to put a label to the AO/MO. If you use the type p you can specify the orbital you want to label in square brackets:

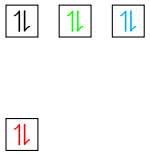
```
\begin{MOdiagram}[style=square]
 \AO{s}[label={s orbital}]{0}
 \AO{p}[label[y]=py,label[z]=pz]{1.5}
\end{MOdiagram}
```



4.3.2 The color Key

Analogous to the label key there is the key color[x/y/z] which enables you to choose a color for the electrons. If you use the type p you can specify the orbital in square brackets:

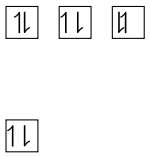
```
\begin{MOdiagram}[style=square]
 \AO{s}[color=red]{0}
 \AO{p}[color[y]=green,color[z]=cyan]{1.5}
\end{MOdiagram}
```



4.3.3 The up-el-pos and down-el-pos Keys

Then there are the keys up-el-pos[x/y/z] and down-el-pos[x/y/z] with which the electrons can be shifted horizontally. You can use values between 0 and 1, also see section 4.1.4. If you use the type p you can specify the orbital in square brackets:

```
\begin{MOdiagram}[style=square]
 \AO{s}[up-el-pos=.15]{0}
 \AO{p}[up-el-pos[y]=.15,down-el-pos[z]=.15]{1.5}
\end{MOdiagram}
```

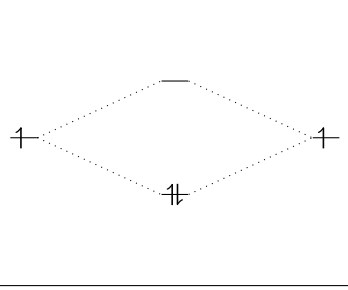


4.4 Energy Axis

Last but not least one might want to add an energy axis to the diagram. For this there is the command \EnergyAxis.

▸ \EnergyAxis[<key = val>]
[<key = val>] key/value pairs to modify the axis.

```
\begin{MOdiagram}
 \atom{left} { 1s = {;up} }
 \atom{right}{ 1s = {;up} }
 \molecule{ 1sMO = {.75;pair} }
 \EnergyAxis
\end{MOdiagram}
```

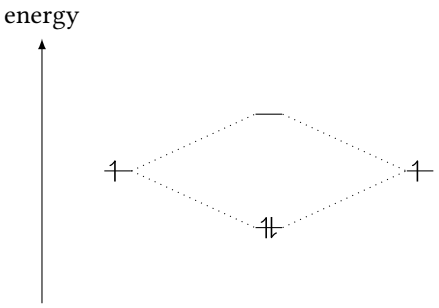


For the time being there are two keys to modify the axis.

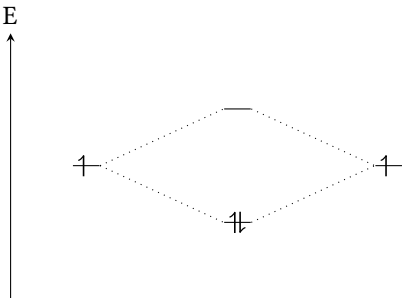
▸ title = <title> ⟶ axis label (default: energy).

▸ head = <tikz-arrow-head> ⟶ arrow head; you can use the arrow heads specified in the Ti*k*Z library arrows (pgfmanual v2.10 pages 256ff.) (default: >).

```
\begin{MOdiagram}
 \atom{left} { 1s = {;up} }
 \atom{right}{ 1s = {;up} }
 \molecule{ 1sMO = {.75;pair} }
 \EnergyAxis[title]
\end{MOdiagram}
```



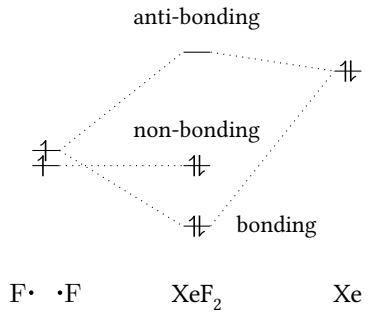

```
\begin{MOdiagram}
 \atom{left} { 1s = {;up} }
 \atom{right}{ 1s = {;up} }
 \molecule{ 1sMO = {.75;pair} }
 \EnergyAxis[title=E,head=stealth]
\end{MOdiagram}
```



5 Examples

The example from the beginning of section 3.4.

```
% use packages ‘chemmacros’ and ‘chemfig’
\begin{MOdiagram}[names]
 \atom[\lewis{0.,F}\hspace*{5mm}\lewis{4.,F}]{left}{1s=.2;up,up-el-
 pos={1sleft=.5}}
 \atom[Xe]{right}{1s=1.25;pair}
 \molecule[\ch{XeF2}]{1sMO={1/.25;pair}}
 \AO(1cm){s}{0;up}
 \AO(3cm){s}{0;pair}
 \connect{ AO1 & AO2 }
 \node[right,xshift=4mm] at (1sigma) {\footnotesize bonding};
 \node[above] at (AO2.90) {\footnotesize non-bonding};
 \node[above] at (1sigma*.90) {\footnotesize anti-bonding};
\end{MOdiagram}
```




```
% use packages ‘chemmacros’ (and ‘textgreek’ loaded by ‘
 modiagram’)
\begin{figure}
 \centering
 \begin{MOdiagram}[style=square,labels,names,AO-width=8pt,
 labels-fs=\footnotesize]
  \atom[\ch{O_a}]{left}{
    1s, 2s, 2p = {;pair,up,up}
  }
  \atom[\ch{O_b}]{right}{
    1s, 2s, 2p = {;pair,up,up}
  }
  \molecule[\ch{O2}]{
    1sMO, 2sMO, 2pMO = {;pair,pair,pair,up,up},
    color = { 2piy*=red, 2piz*=red }
  }
  \EnergyAxis
 \end{MOdiagram}
 \caption{MO diagram of \ch{^3 "\textSigma-" O2}.}
\end{figure}
```

```
% use package ‘chemfig’
\begin{figure}
 \centering\MOsetup{style = fancy, distance = 7cm, AO-width
  = 15pt, labels}
 \begin{MOdiagram}
  \atom[N]{left}{
    2p = {0;up,up,up}
  }
  \atom[O]{right}{
    2p = {2;pair,up,up}
  }
  \molecule[NO]{
    2pMO = {1.8,.4;pair,pair,pair,up},
    color = { 2piy*=red }
  }
```

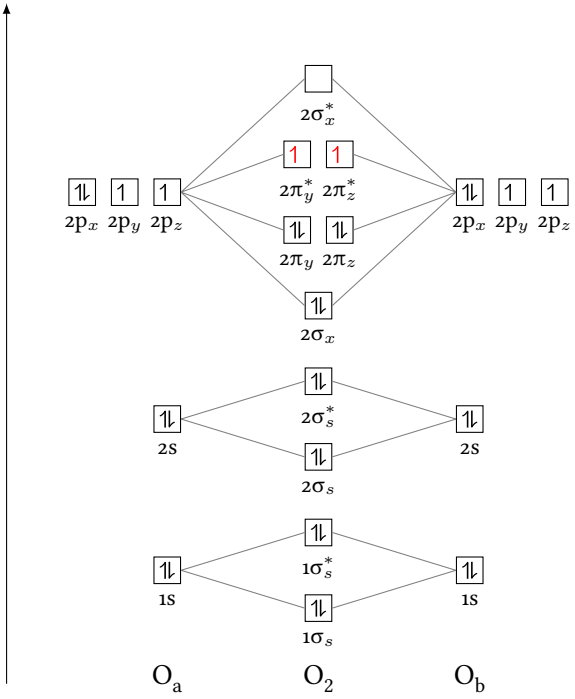


Figure 1: MO diagram of $^3\Sigma$-O_2.

```
    \EnergyAxis
  \end{MOdiagram}
  \caption{Part of the MO diagram of \protect\Lewis{4.,NO}.}
 \end{figure}
```

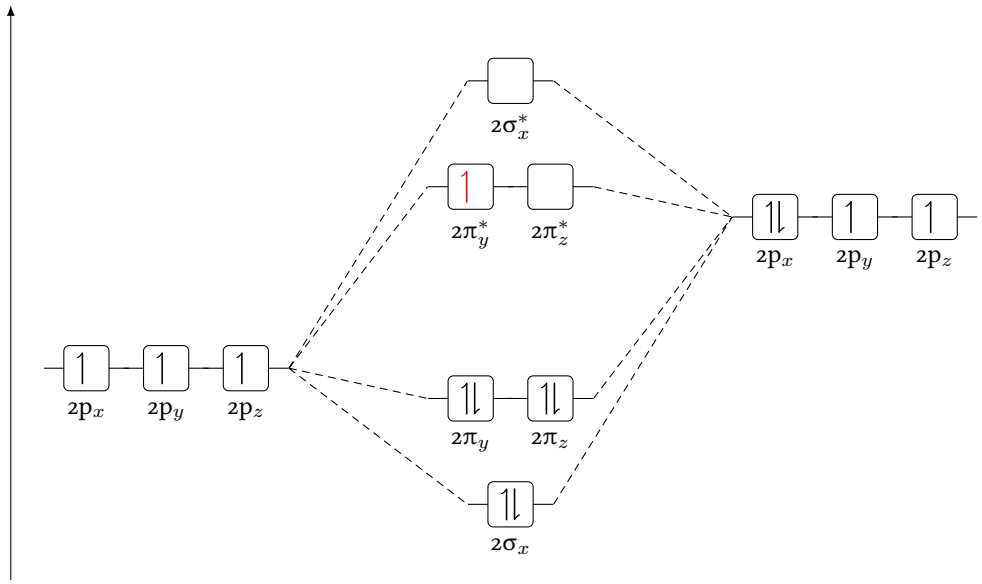


Figure 2: Part of the MO diagram of •NO.

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