MOdiagram v0.1

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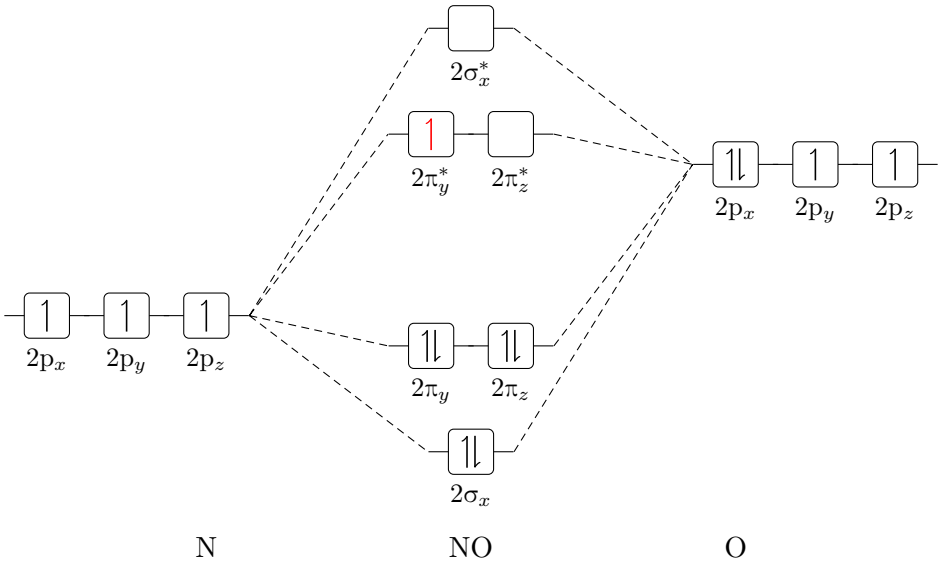
MOdiagram provides an environment and commands for the creation of molecular orbital diagrams.



Contents

1 Licence, Requirements

MOdiagram v0.1 underlies the LaTeX Project Public License version 1.3 or later. (http://www.latex-project.org/lppl.txt)

MOdiagram needs the packages expl3[1], xparse[2], l3keys2e[3], tikz[4], amsmath[5] and textgreek[6]. Additionally the TikZ libraries calc and arrows are loaded.

It is useful to be familiar with the pgf[7] or the tikz[8] package.

[1] http://www.ctan.org/pkg/expl3/
[2] http://www.ctan.org/pkg/xparse/
[3] http://www.ctan.org/pkg/l3keys2e/
[4] http://www.ctan.org/pkg/pgf/
[5] http://www.ctan.org/pkg/amsmath/
[6] http://www.ctan.org/pkg/textgreek/
[7] http://www.ctan.org/pkg/pgf/
[8] http://www.ctan.org/pkg/tikz/

2 Motivation

This package has been written as a reaction to a question on http://tex.stackexchange.com/. To be more precise: as a rection 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 TikZ.*

The problem was solved using TikZ, since no package existed for that purpose. MOdiagram is intended to fill this gap.

3 Main Commands

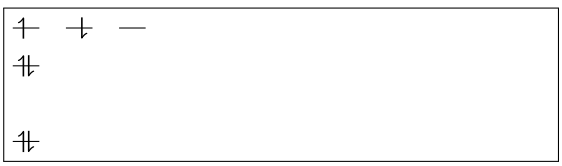
Every molecular orbital (MO) diagrams are created using the environment `MOdiagram` . Inside this environment two commands are important to begin with.

3.1 The `\atom` Command

`\atom[<name>]{<pos>}{<AO-spec>}`

- `<name>` (o) caption of the atom
- `<pos>` (m) on the left or the right in the diagram
- `<AO-spec>` (m) specifications of the atomic orbitals (AO)

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 ansd shifts the AO vertically by `<rel. energy>` cm.

The argument `<pos>` 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 canbe adjusted individually, see page 13.

```
\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}
```

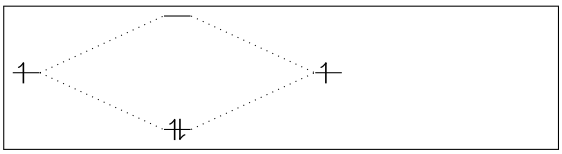
With the next command the reason for the shift becomes clear.

3.2 The `\molecule` command

`\molecule[<name>]{<MO-spec>}`

- `<name>` (o) caption of the molekule
- `<MO-spec>` (m) specifications of the molecular orbitals (MO)

An example first:



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

The command `\molecule` connects the AO with the bonding and anti-bondung MO. `\molecule` can only be used *after* one has set *both* atoms, since the orbitals, that should be connected, must be known.

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

- `1sMO={<energy gain>; <s el-spec>, <s* el-spec>}` (connects the AO specified by `1s`)
- `2sMO={<energy gain>; <s el-spec>, <s* el-spec>}` (connects the AO specified by `2s`)
- `2pMO={<s energy gain>, <p energy gain>; <s el-spec>, <py el-spec>, <pz el- spec>, <py* el-spec>, <pz* el-spec>, <s* el-spec>}` (connects the AO specified by `2p`)

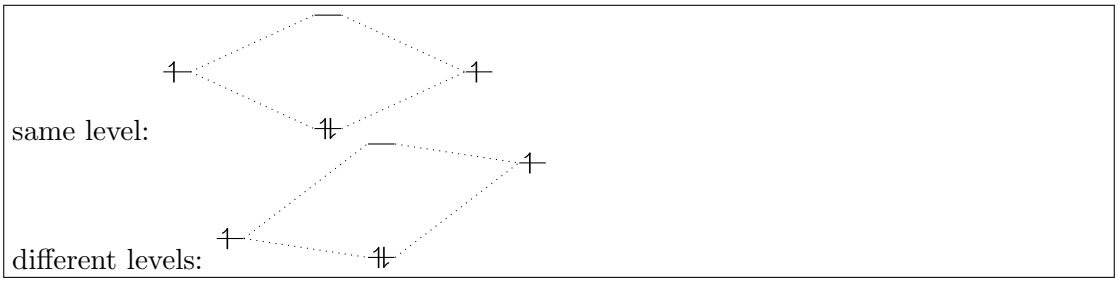
Obviously the regarding AO must have been set in order to connect them. This for example won't work:

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

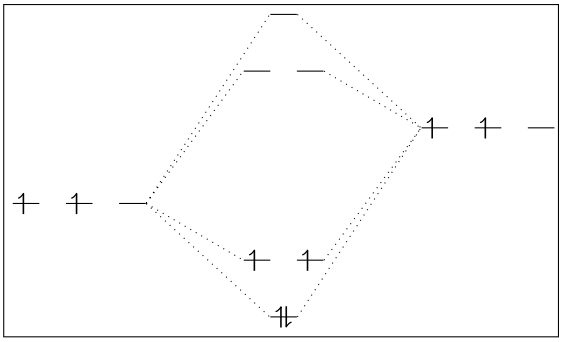
The value used in `<energy gain>` determines how many cm the bonding MO lies below the lower AO or how many cm the anti-bondung MO lies above the higher AO.

```
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}
```

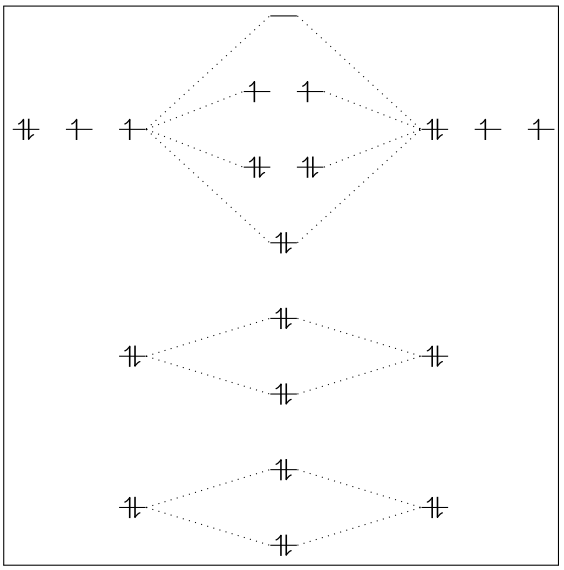


Please be aware, that you have to specify *two* such values with `2pMO`: the splitting of the σ orbitals and the splitting of the π orbitals.



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

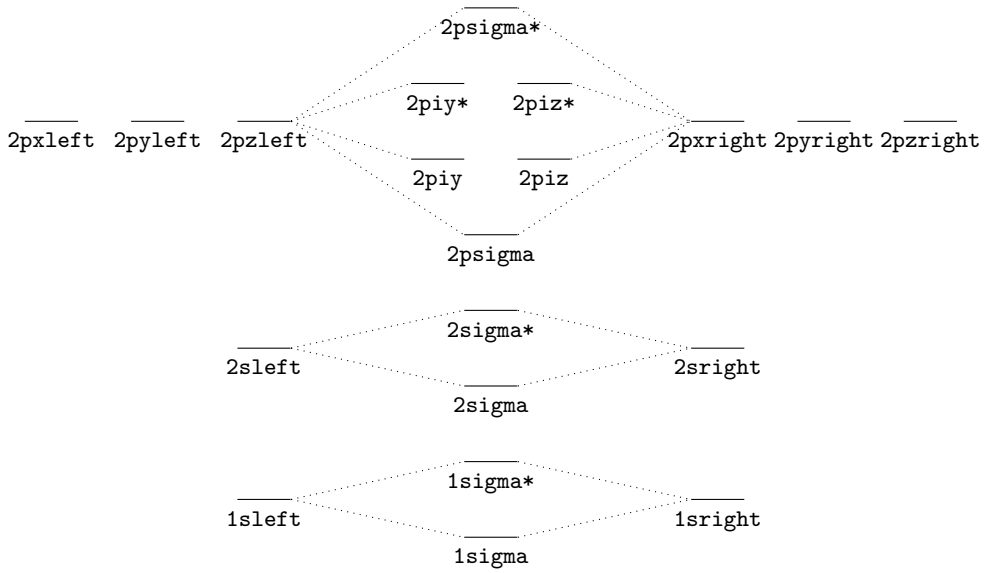
The complete MO diagram for triplett dioxygen now could look something like that:



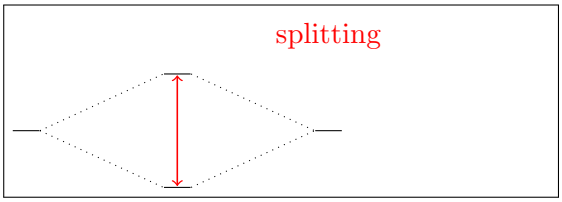
```
\begin{MOdiagram}
 \atom{left}{
   1s = {0;pair},
   2s = {2;pair},
   2p = {5;pair,up,up}
 }
 \atom{right}{
   1s = {0;pair},
   2s = {2;pair},
   2p = {5;pair,up,up}
 }
 \molecule{
   1sMO  = {.5;pair,pair},
   2sMO  = {.5;pair,pair},
   2pMO  = {1.5,.5;pair,pair,pair,up
       ,up,}
 }
\end{MOdiagram}
```

3.3 The Naming Scheme

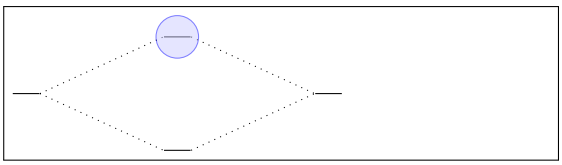
Since one wants to be able to put labels to the orbitals and since they are nodes in a tikzpicture, the internal naming scheme is important. It closely follows the function:



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



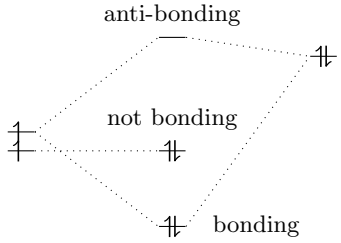

```
\begin{MOdiagram}
 \atom{left} { 1s = {0; } }
 \atom{right}{ 1s = {0; } }
 \molecule { 1sMO = {.75; , } }
 \draw[<->,red,semithick] (1sigma)
     -- (1sigma*) ;
 \draw[red] (1sigma*) ++ (2cm,.5cm)
     node {splitting} ;
\end{MOdiagram}
```



```
\begin{MOdiagram}
 \atom{left} { 1s = {0; } }
 \atom{right}{ 1s = {0; } }
 \molecule { 1sMO = {.75; , } }
 \draw[draw=blue,fill=blue!20,
     opacity=.5] (1sigma*) circle (8
     pt);
\end{MOdiagram}
```

3.4 Placing AO and MO 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 this part, that illustrates the interaction between the bonding and anti-bonding combination of two p orbitals of Flourine with one p orbital of Xenon:



$F\cdot \quad \cdot F \qquad XeF_2 \qquad Xe$

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

`\AO[<name>](<xshift>){<type>}{<energy>;<el-spec>}`

- `<name>` (o) name of the node
- `<xshift>` (o) vertical position of the Orbitals, a TEX dimension.
- `<type>` (m) `s` or `p`
- `<AO-spec>` (m) specification of the AO

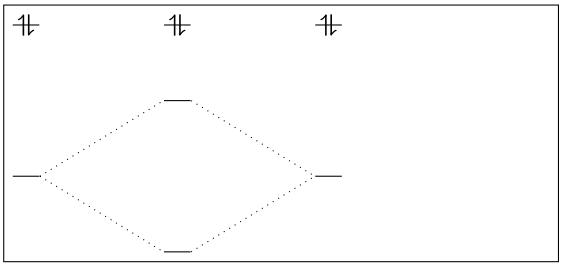
Depending on the <type> one s or three p porbitals are drawn.

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

Please notice, that <el-spec> only awaits one specification with the type s, but three with the type p, separated with commas.

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

- atom left: 1 cm
- molecule: 3 cm
- atom right: 5 cm

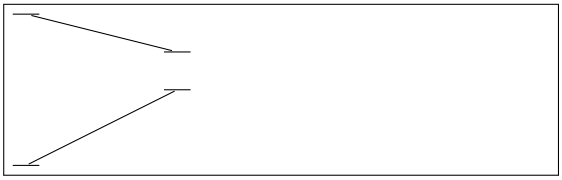


```
\begin{MOdiagram}
 \atom{left} {1s={0;}}
 \atom{right}{1s={0;}}
 \molecule {1sMO={1;,}}
 \AO(1cm){s}{2;pair}
 \AO(3cm){s}{2;pair}
 \AO(5cm){s}{2;pair}
\end{MOdiagram}
```

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

The AO created with \AO also can be connected. For this you can use the Ti*k*Z command \draw, of course:



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

However, if you want the lines to be drawn in the same style as the ones created by `\molecule`[9], you should use the command `\connect`.

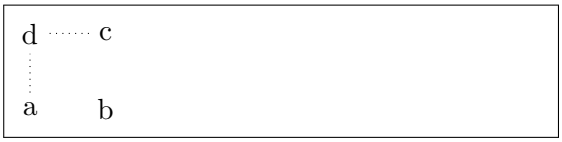
`\connect{<AO-connect>}`

- `<AO-connect>` (m) 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[a]{s}{0;} \AO[b](2cm){s}{1;}
 \AO[c]{s}{2;} \AO[d](2cm){s}{1.5;}
 \connect{ a & b, c & d }
\end{MOdiagram}
```

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:

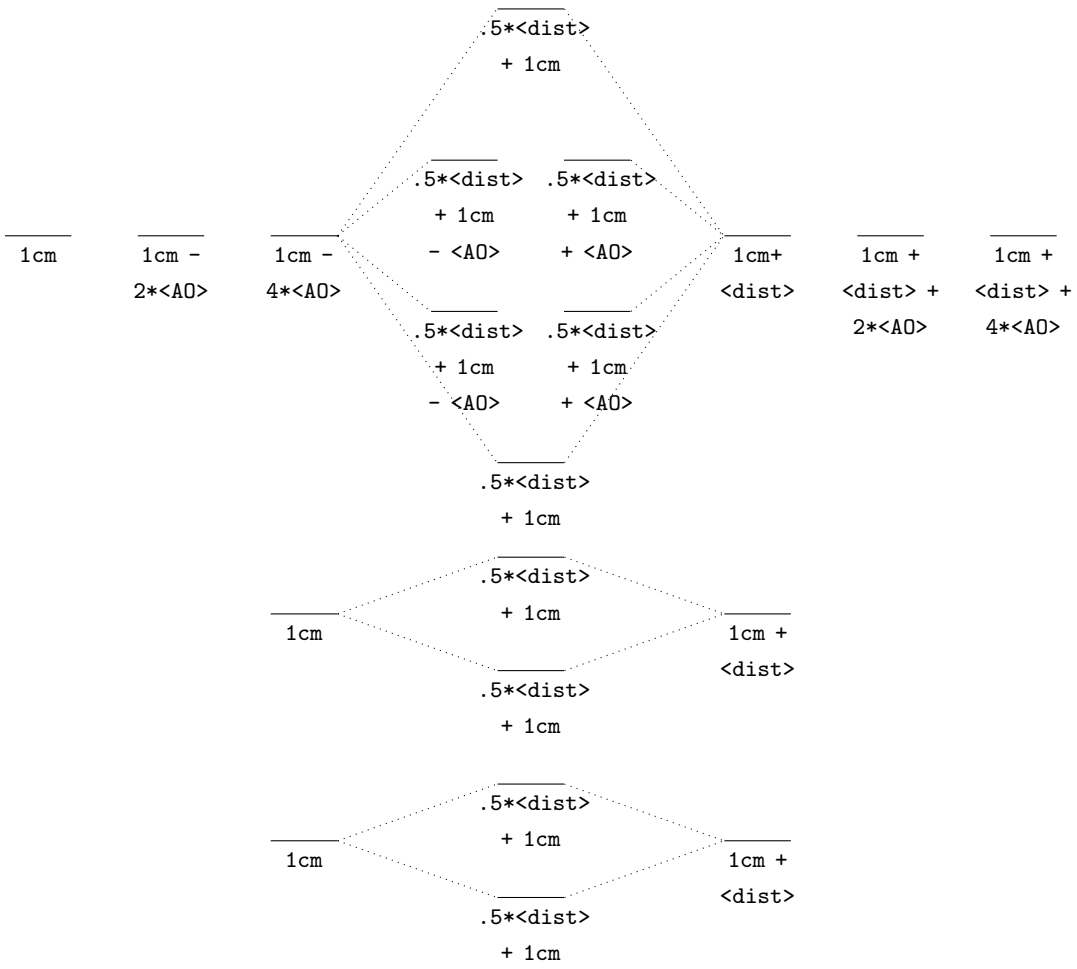



```
\begin{tikzpicture}
 \draw (0,0) node (a) {a} ++ (1,0)
     node (b) {b}
       ++ (0,1) node (c) {c} ++
           (-1,0) node (d) {d} ;
 \connect{ a.90 & d.-90, c.180 & d.0
      }
\end{tikzpicture}
```

3.5 The Positioning Scheme

The figure below shows the values of the x coordinates of the orbitals, depending in 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.

[9] which can be customized, see page 14



4 Customization

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.
- `lines=<tikz>` change the Ti*k*Z style of the connecting lines, section 4.1.4.
- `names=<bool>` add captions to the atoms and the molecule, section 4.1.5.
- `labels=<bool>` add default labels to the orbitals, section 4.1.6.

- `labels-fs=<cs>` change the font size of the labels, section 4.1.7.
- `labels-style=<tikz>` change the Ti*k*Z style of the labels, section 4.1.8.

They all are discussed in the following sections. They are used either as option of the environment

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

or as argument of the setup command

`\MOsetup{<key = value>}`

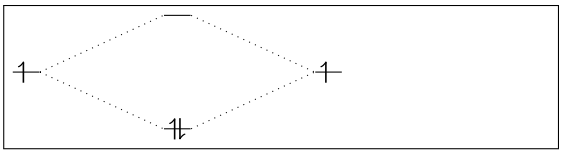
- `<key = val>` (m) comma separated key/value list

4.1.1 Option `style`

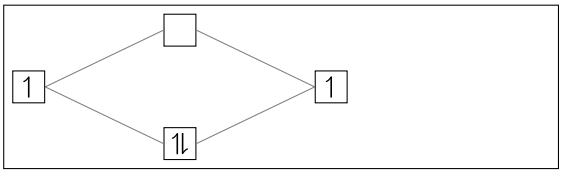
There are four different styles, which can be chosen.

- `style=plain` ↿⇂ (default)
- `style=square` 1
- `style=round` 1
- `style=fancy` 1

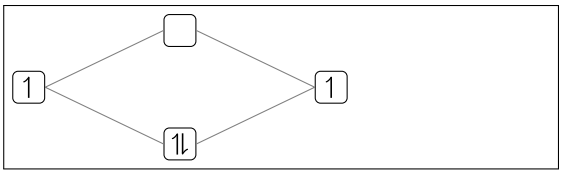
Let's take the MO diagram of H_2 to illustrate the different styles:



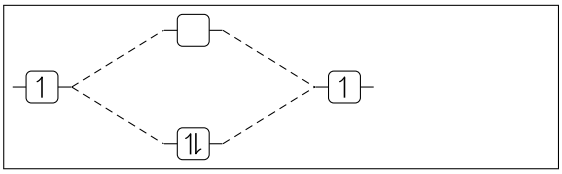
```
% use package 'mhchem'
\begin{MOdiagram}[style=plain]%
    Default
 \atom[H]{left} { 1s = {0;up} }
 \atom[H]{right}{ 1s = {0;up} }
 \molecule[\ce{H2}]{ 1sMO = {.75;
     pair,} }
\end{MOdiagram}
```



```
% use package 'mhchem'
\begin{MOdiagram}[style=square]
 \atom[H]{left} { 1s = {0;up} }
 \atom[H]{right}{ 1s = {0;up} }
 \molecule[\ce{H2}]{ 1sMO = {.75;
     pair,} }
\end{MOdiagram}
```



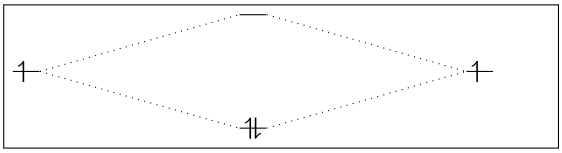
```
% use package 'mhchem'
\begin{MOdiagram}[style=round]
 \atom[H]{left} { 1s = {0;up} }
 \atom[H]{right}{ 1s = {0;up} }
 \molecule[\ce{H2}]{ 1sMO = {.75;
     pair,} }
\end{MOdiagram}
```



```
% use package 'mhchem'
\begin{MOdiagram}[style=fancy]
 \atom[H]{left} { 1s = {0;up} }
 \atom[H]{right}{ 1s = {0;up} }
 \molecule[\ce{H2}]{ 1sMO = {.75;
     pair,} }
\end{MOdiagram}
```

4.1.2 Option `distance`

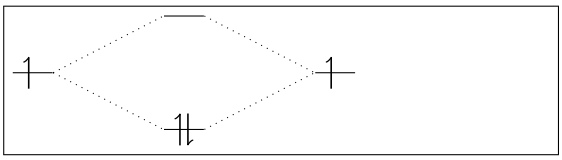
Depending on labels and captions the 4 cm by which the right and left atom are separated can be too small. With `distance=<dim>` the length can be adjusted. With this, the position of the right atom is changed to `1cm + <dim>` and the position of the molecule is changed to `0.5*(1cm + <dim>)`, also see page Seite 9 and section 3.5.



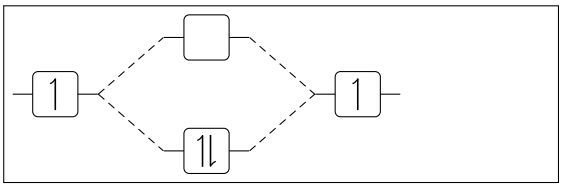
```
% use package 'mhchem'
\begin{MOdiagram}[distance=6cm]
 \atom[H]{left} { 1s = {0;up} }
 \atom[H]{right}{ 1s = {0;up} }
 \molecule[\ce{H2}]{ 1sMO = {.75;
     pair,} }
\end{MOdiagram}
```

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 'mhchem'
\begin{MOdiagram}[AO-width=15pt]
 \atom[H]{left} { 1s = {0;up} }
 \atom[H]{right}{ 1s = {0;up} }
 \molecule[\ce{H2}]{ 1sMO = {.75;
     pair,} }
\end{MOdiagram}
```

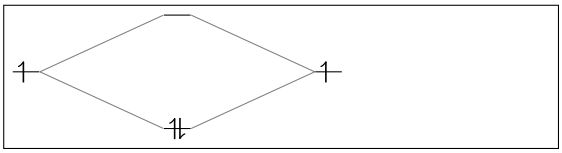


```
% use package 'mhchem'
\begin{MOdiagram}[style=fancy,AO-
    width=15pt]
 \atom[H]{left} { 1s = {0;up} }
 \atom[H]{right}{ 1s = {0;up} }
 \molecule[\ce{H2}]{ 1sMO = {.75;
    pair,} }
\end{MOdiagram}
```

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 Option `lines`

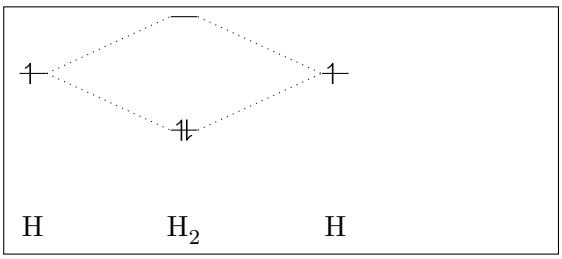
The option `lines` can be used to modify the Ti*k*Z style of the connecting lines:



```
% use package 'mhchem'
\begin{MOdiagram}[lines={gray,thin
    }]
 \atom[H]{left} { 1s = {0;up} }
 \atom[H]{right}{ 1s = {0;up} }
 \molecule[\ce{H2}]{ 1sMO = {.75;
    pair,} }
\end{MOdiagram}
```

4.1.5 Option `names`

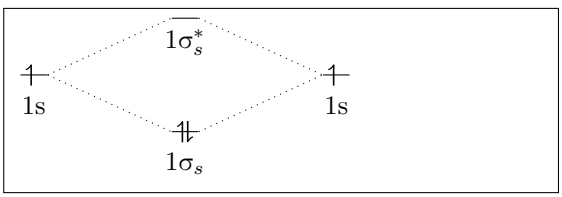
If you use the option `names`, the atoms and the molecule get captions, if you have used the optional `<name>` argument of `\atom` and/or `\molecule`.




```
% use package 'mhchem'
\begin{MOdiagram}[names]
 \atom[H]{left} { 1s = {0;up} }
 \atom[H]{right}{ 1s = {0;up} }
 \molecule[\ce{H2}]{ 1sMO = {.75;
    pair,} }
\end{MOdiagram}
```

4.1.6 Option `labels`

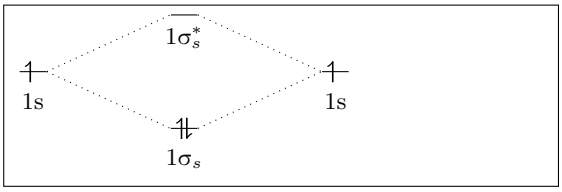
If you use the option `labels`, predefined labels are written below the orbitals. These labels can be changed, see section 4.2.1.




```
% use package 'mhchem'
\begin{MOdiagram}[labels]
 \atom[H]{left} { 1s = {0;up} }
 \atom[H]{right}{ 1s = {0;up} }
 \molecule[\ce{H2}]{ 1sMO = {.75;
    pair,} }
\end{MOdiagram}
```

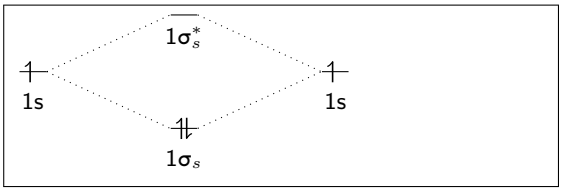
4.1.7 Option `labels-fs`

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




```
% use package 'mhchem'
\begin{MOdiagram}[labels,labels-fs
    =\footnotesize]
 \atom[H]{left} { 1s = {0;up} }
 \atom[H]{right}{ 1s = {0;up} }
 \molecule[\ce{H2}]{ 1sMO = {.75;
     pair,} }
\end{MOdiagram}
```

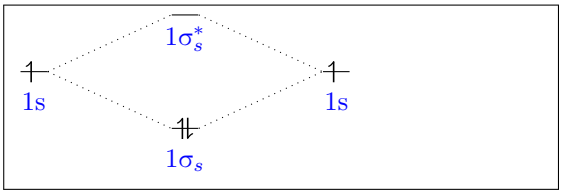
This also allows you to change the font style or font shape of the labels.




```
% use package 'mhchem'
\begin{MOdiagram}[labels,labels-fs
    =\sffamily\footnotesize]
 \atom[H]{left} { 1s = {0;up} }
 \atom[H]{right}{ 1s = {0;up} }
 \molecule[\ce{H2}]{ 1sMO = {.75;
     pair,} }
\end{MOdiagram}
```

4.1.8 Option `labels-style`

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

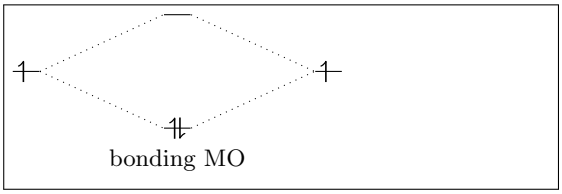



```
% use package 'mhchem'
\begin{MOdiagram}[labels,labels-
    style={blue}]
 \atom[H]{left} { 1s = {0;up} }
 \atom[H]{right}{ 1s = {0;up} }
 \molecule[\ce{H2}]{ 1sMO = {.75;
     pair,} }
\end{MOdiagram}
```

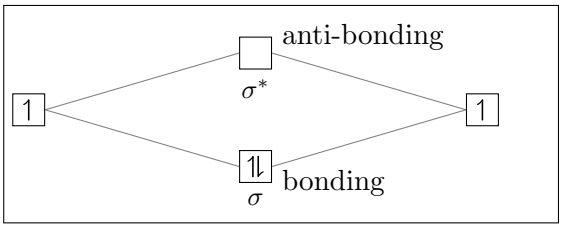
4.2 `\atom` and `\molecule` Specific Customizations

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.



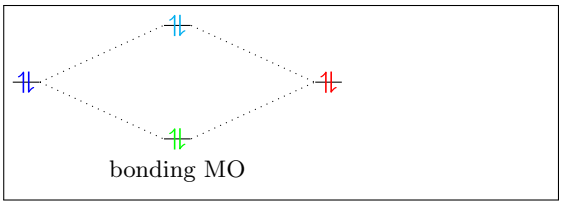

```
% use package 'mhchem'
\begin{MOdiagram}[labels-fs=\
    footnotesize]
 \atom[H]{left} { 1s = {0;up} }
 \atom[H]{right}{ 1s = {0;up} }
 \molecule[\ce{H2}]{
   1sMO  = {.75;pair,},
   label = { 1sigma = {bonding MO} }
 }
\end{MOdiagram}
```




```
\begin{MOdiagram}[style=square,
    distance=6cm]
 \atom{left} { 1s = {0;up} }
 \atom{right}{ 1s = {0;up} }
 \molecule{
   1sMO  = {.75;pair,} ,
   label = {
     1sigma = $\sigma$,
     1sigma* = $\sigma^*$
   }
 }
 \node[right] at (1sigma.-45) {
    bonding};
 \node[right] at (1sigma*.45) {anti-
    bonding};
\end{MOdiagram}
```

4.2.2 The `color` Key

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



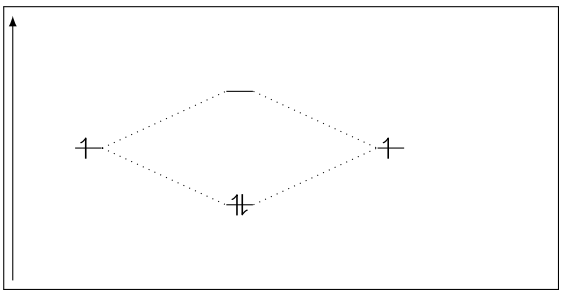

```
% use package 'mhchem'
\begin{MOdiagram}[labels-fs=\
    footnotesize]
 \atom[H]{left}{
   1s = {0;pair},
   color = { 1sleft = blue }
 }
 \atom[H]{right}{
   1s = {0;pair},
   color = { 1sright = red }
 }
 \molecule[\ce{H2}]{
   1sMO  = {.75;pair,pair},
   label = { 1sigma = {bonding MO}
       },
   color = { 1sigma = green, 1sigma*
       = cyan }
 }
\end{MOdiagram}
```

4.3 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>]`

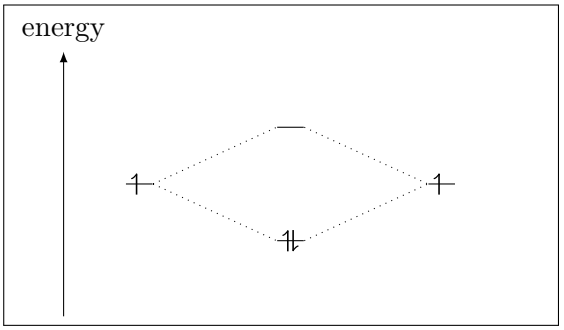
- `<key = val>` (o) key/value pairs to modify the axis



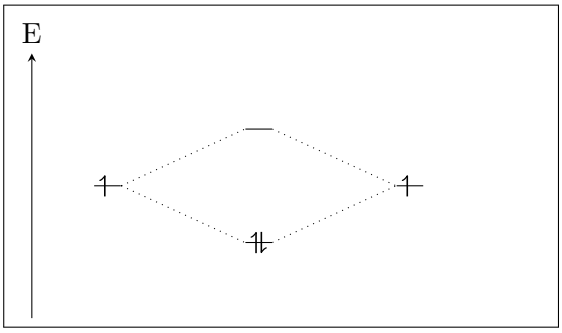
```
\begin{MOdiagram}
 \atom{left} { 1s = {0;up} }
 \atom{right}{ 1s = {0;up} }
 \molecule{ 1sMO = {.75;pair,} }
 \EnergyAxis
\end{MOdiagram}
```

For the time beeing 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[10] (pgfmanual v2.10 pages 256ff.) (default: `>`).




```
\begin{MOdiagram}
 \atom{left} { 1s = {0;up} }
 \atom{right}{ 1s = {0;up} }
 \molecule{ 1sMO = {.75;pair,} }
 \EnergyAxis[title]
\end{MOdiagram}
```




```
\begin{MOdiagram}
 \atom{left} { 1s = {0;up} }
 \atom{right}{ 1s = {0;up} }
 \molecule{ 1sMO = {.75;pair,} }
 \EnergyAxis[title=E,head=stealth]
\end{MOdiagram}
```

4.4 Examples

```
% use packages 'mhchem' (and 'textgreek' loaded by 'MOdiagram')
\begin{figure}
 \centering
 \begin{MOdiagram}[style=square,labels,names,AO-width=8pt,labels-fs=\
     footnotesize]
  \atom[\ce{O_a}]{left}{
    1s = {0;pair},
    2s = {2;pair},
    2p = {5;pair,up,up}
  }
  \atom[\ce{O_b}]{right}{
    1s = {0;pair},
    2s = {2;pair},
    2p = {5;pair,up,up}
  }
  \molecule[\ce{O2}]{
    1sMO  = {.5;pair,pair},
    2sMO  = {.5;pair,pair},
    2pMO  = {1.5,.5;pair,pair,pair,up,up,},
    color = { 2piy*=red, 2piz*=red }
  }
  \EnergyAxis
 \end{MOdiagram}
 \caption{MO diagram of $^3$\textSigma-\ce{O2}.}
\end{figure}
```

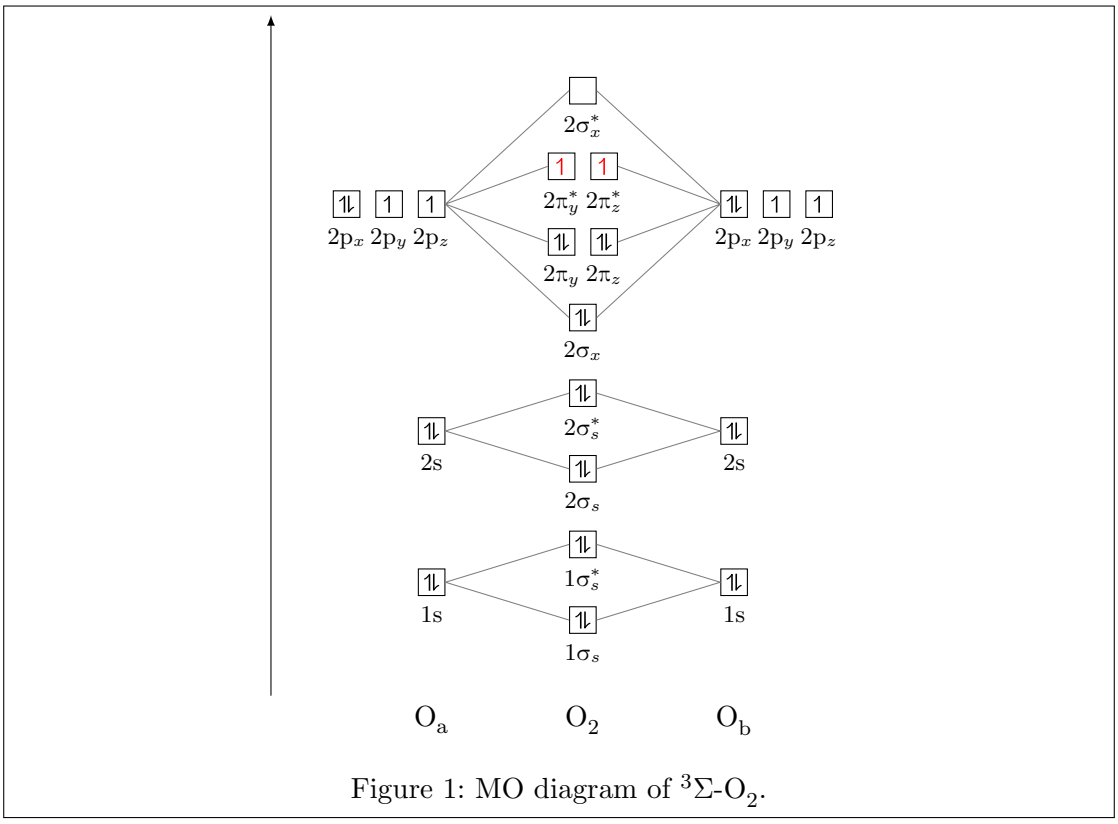


Figure 1: MO diagram of $^3\Sigma$-O_2.

```
% use package 'chemfig'
\begin{figure}
 \centering
 \begin{MOdiagram}[style=fancy,distance=7cm,AO-width=15pt,labels]
  \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 }
  }
  \EnergyAxis[title]
 \end{MOdiagram}
 \caption{Part of the MO diagram of \protect\Lewis{4.,NO}.}
\end{figure}
```

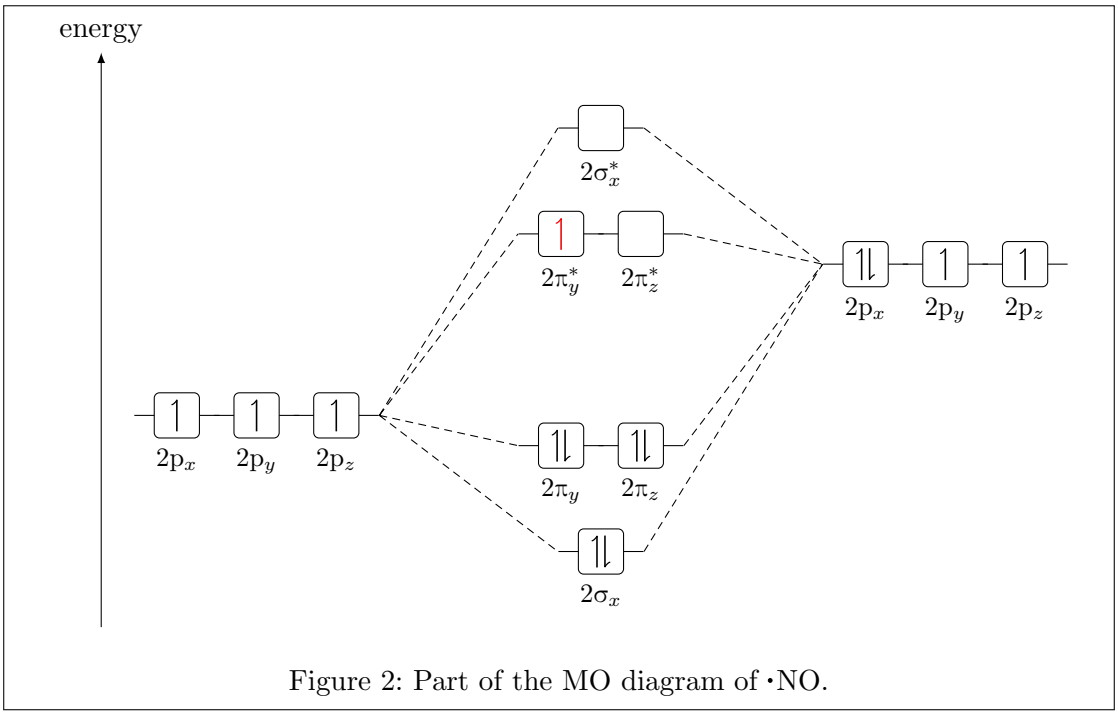


Figure 2: Part of the MO diagram of ·NO.