

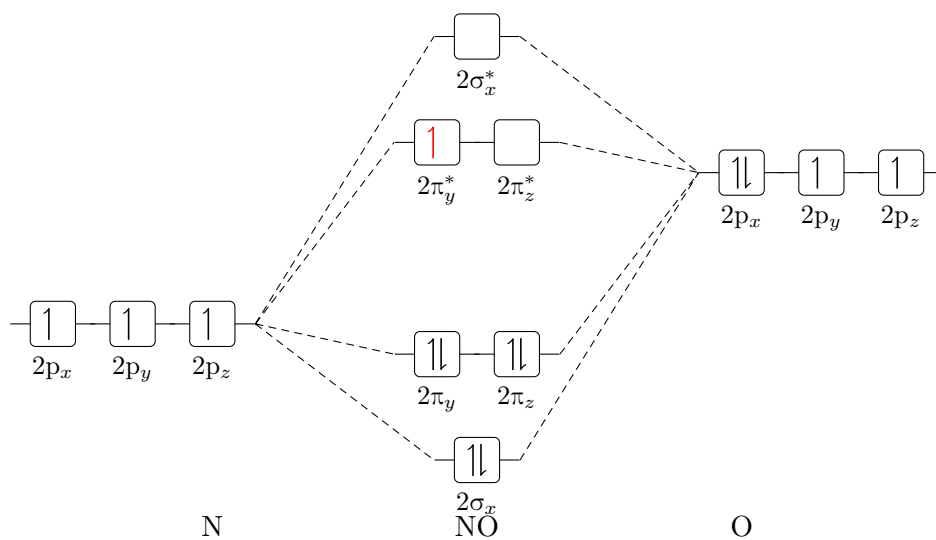
MOdiagram v0.2

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



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1 Licence, Requirements

MOdiagram v0.2 underlies the L^AT_EX 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 and `textgreek`⁵. Additionally the `TikZ` libraries `calc` and `arrows` are loaded.

Knowledge of `pgf` or `tikz` would be useful.

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 L^AT_EX](#). There it says

I'm wondering if anyone has seen a package for drawing (qualitative) molecular orbital splitting diagrams in L^AT_EX? 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. 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 `MOdiagram`. When the commands are described in the following sections, arguments are marked with (o) or (m) meaning *optional* or *mandatory* argument.

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)

¹<http://www.ctan.org/pkg/expl3>

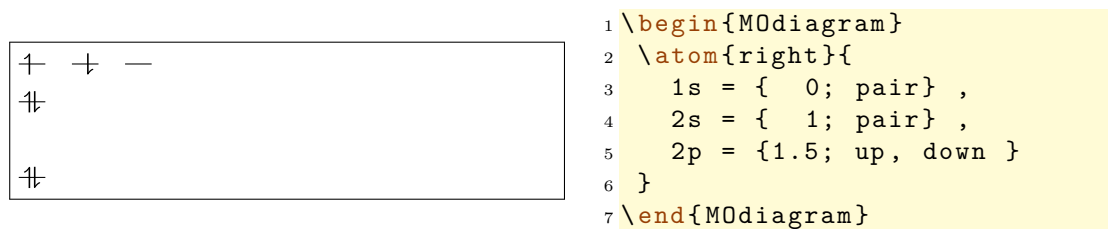
²<http://www.ctan.org/pkg/xparse>

³<http://www.ctan.org/pkg/l3keys2e>

⁴<http://www.ctan.org/pkg/pgf>

⁵<http://www.ctan.org/pkg/textgreek>

Let's take a look at an example:

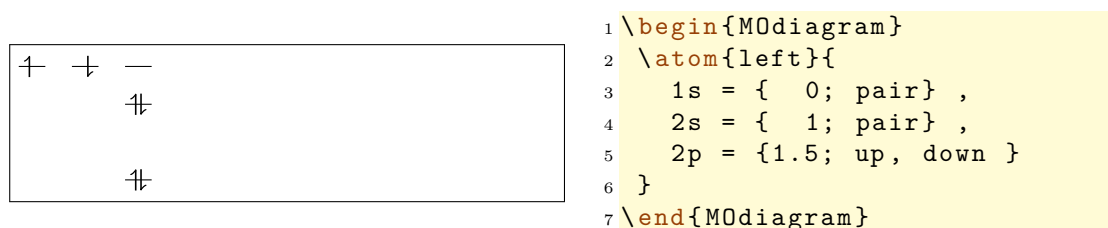


As you can see, the argument `<AO-spec>` is essential to create the actual orbitals and the electrons within. You can use these key/value pairs to specify what you need:

- `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 `<pos>` is important, when p orbitals are used. For instance compare the following example to the one before:

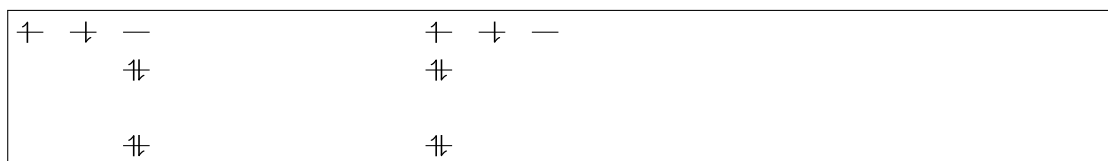


When both variants are used one can also see, that the right atom is shifted to the right (hence the naming). The right atom is shifted by 4 cm per default and can be adjusted individually, see page [17](#).

```

1 \begin{M0diagram}
2   \atom{left}{
3     1s = { 0; pair} ,
4     2s = { 1; pair} ,
5     2p = {1.5; up, down }
6   }
7   \atom{right}{
8     1s = { 0; pair} ,
9     2s = { 1; pair} ,
10    2p = {1.5; up, down }
11  }
12 \end{M0diagram}

```



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

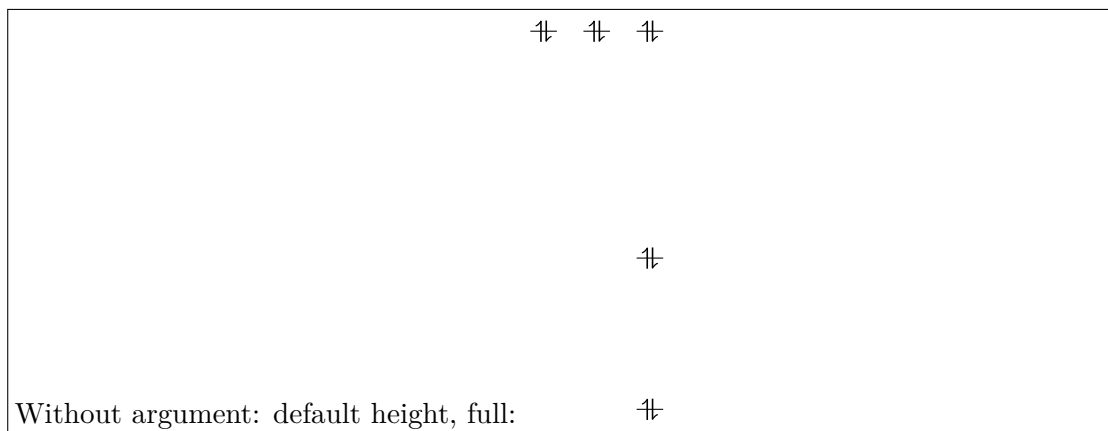
NEW

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

```

1 Without argument: default height, full:
2 \begin{M0diagram}
3   \atom{left}{1s, 2s, 2p}
4 \end{M0diagram}

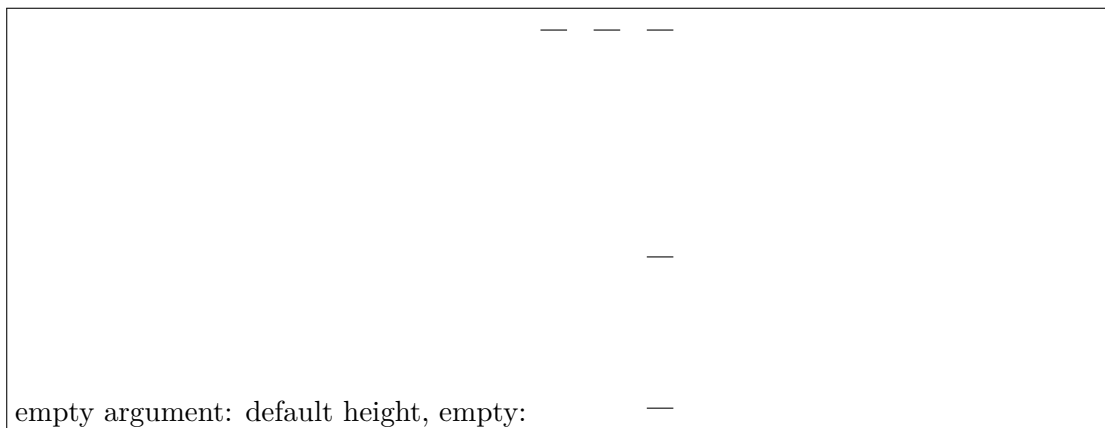
```



```

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

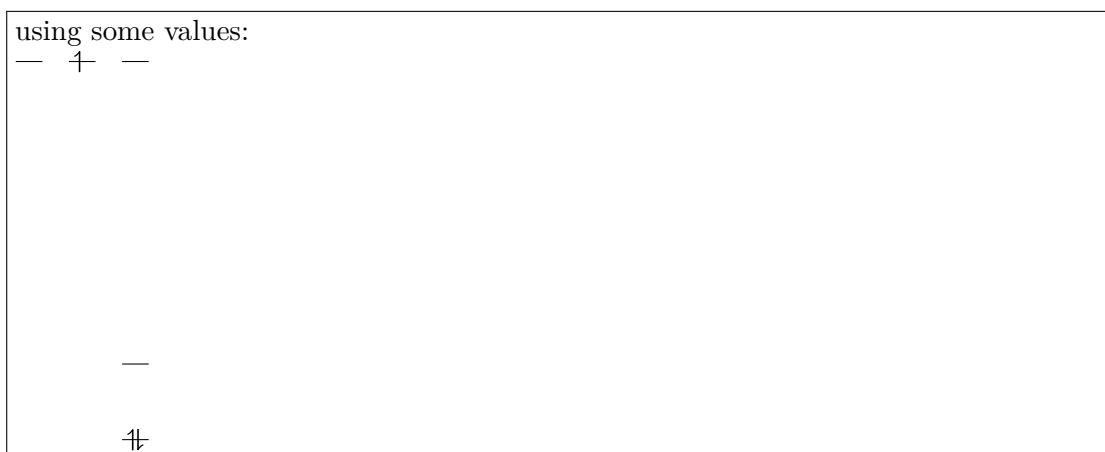
```



```

1 using some values:\\
2 \begin{MOdiagram}
3   \atom{left}{1s, 2s=1, 2p={;,up} }
4 \end{MOdiagram}

```

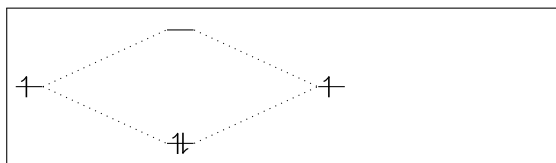


3.2 The `\molecule` Command

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

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

An example first:



```

1 \begin{MOdiagram}
2 \atom{left} { 1s = { 0; up
3 \atom{right}{ 1s = { 0; up
4 \molecule { 1sMO = {.75;
5 \end{MOdiagram}

```

The command `\molecule` connects the AO with the bonding and anti-bonding 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>/<energy loss>; <s el-spec>, <s* el-spec>}`
(connects the AO specified by 1s)
- `2sMO={<energy gain>/<energy loss>; <s el-spec>, <s* el-spec>}`
(connects the AO 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 AO specified by 2p)

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

```

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

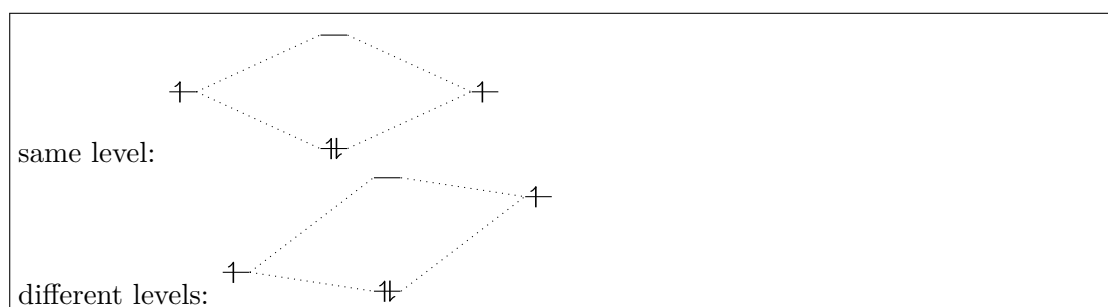
```

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

```

1 same level:
2 \begin{MOdiagram}
3   \atom{left} { 1s = { 0; up } }
4   \atom{right}{ 1s = { 0; up } }
5   \molecule { 1sMO = {.75; pair } }
6 \end{MOdiagram}
7
8 different levels:
9 \begin{MOdiagram}
10  \atom{left} { 1s = { 0; up } }
11  \atom{right}{ 1s = { 1; up } }
12  \molecule { 1sMO = {.25; pair } }
13 \end{MOdiagram}

```

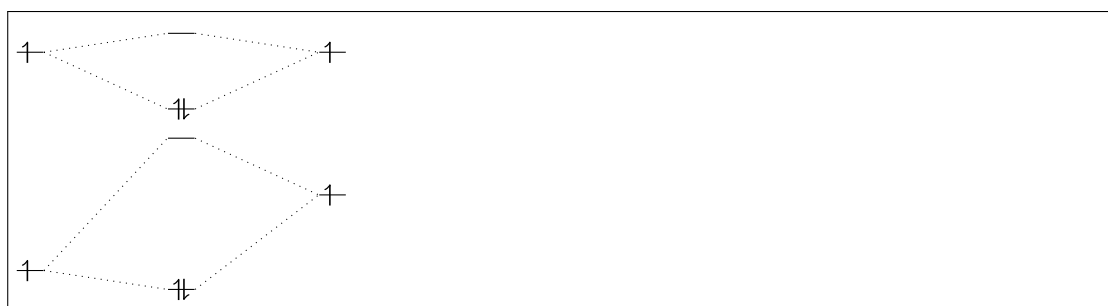


NEW If you specify <energy loss>, you can create non-symmetrical splittings. Then, the first value (<energy gain>) is used for the bonding MO and the second value (<energy loss>) is used for the anti-bonding MO.

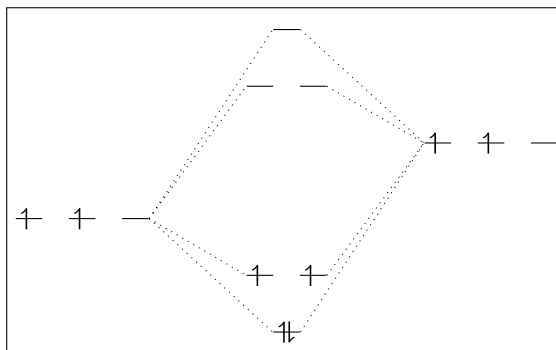
```

1 \begin{MOdiagram}
2   \atom{left} { 1s = { 0; up } }
3   \atom{right}{ 1s = { 0; up } }
4   \molecule { 1sMO = {.75/.25; pair } }
5 \end{MOdiagram}
6
7 \begin{MOdiagram}
8   \atom{left} { 1s = { 0; up } }
9   \atom{right}{ 1s = { 1; up } }
10  \molecule { 1sMO = {.25/.75; pair } }
11 \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.

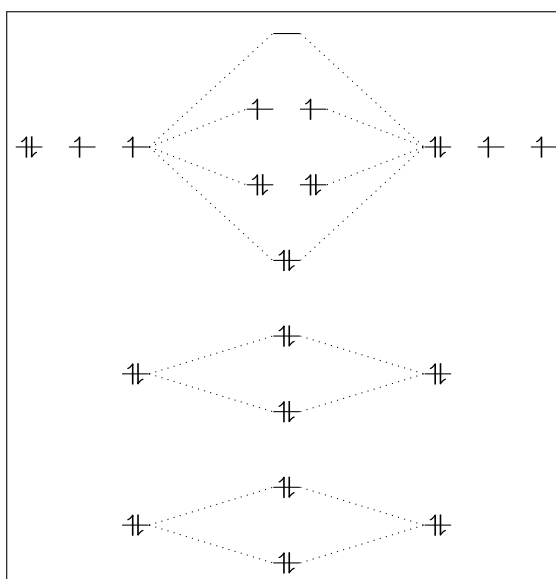


```

1 \begin{MOdiagram}
2 \atom{left}{ { 2p = { 0; up,
3   up } } }
4 \atom{right}{ { 2p = { 1; up,
5   up } } }
6 \molecule { 2pMO = { 1.5,
7   .75; pair, up, up } }
8 \end{MOdiagram}

```

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



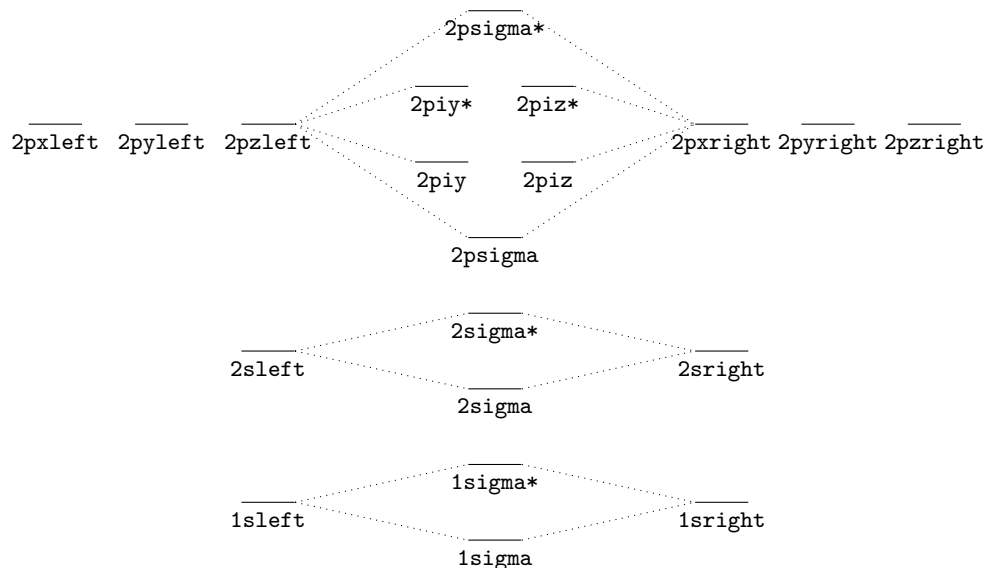
```

1 \begin{MOdiagram}
2 \atom{left}{
3   1s, 2s, 2p = {;pair,up,up}
4 }
5 \atom{right}{
6   1s, 2s, 2p = {;pair,up,up}
7 }
8 \molecule{
9   1sMO, 2sMO, 2pMO = {;pair,
10    pair,pair,up,up}
11 }
12 \end{MOdiagram}

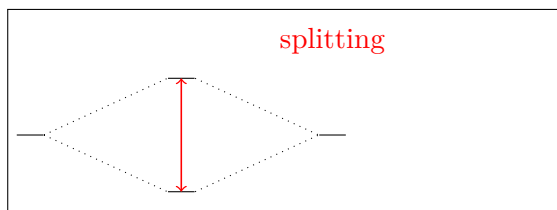
```

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:



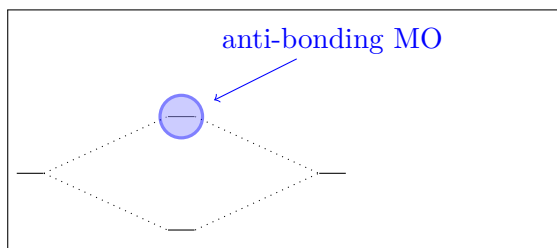
With these names it is possible to reference the orbitals with the known TikZ commands:



```

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

```



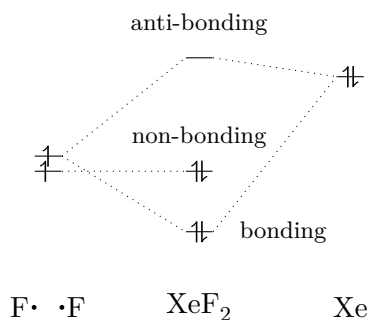
```

1 \begin{MOdiagram}
2 \atom{left} { 1s = 0 }
3 \atom{right}{ 1s = 0 }
4 \molecule { 1sMO = .75 }
5 \draw[draw=blue,very thick,
   fill=blue!40,opacity=.5]
   (1sigma*) circle (8pt);
6 \draw[<->,shorten <=8pt,
   shorten >=15pt,blue] (1
   sigma*) --++(2,1) node {
   anti-bonding MO};
7 \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:



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> (o) name of the node; if not specified, $\text{AO}\#$ is used where # is a consecutive number.
- <xshift> (o) vertical position of the orbitals, a $\text{T}_{\text{E}}\text{X}$ dimension.
- <type> (m) s or p
- <key = val> (o) key/value pairs, with which the AO can be customized, see section 4.3.
- <AO-spec> (m) specification of the AO

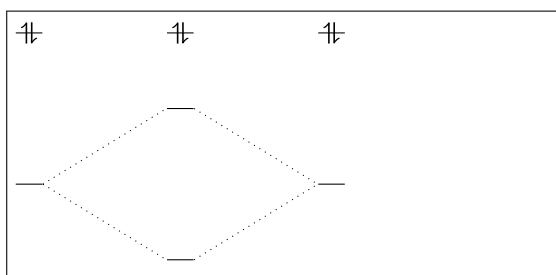
Depending on the <type> one s or three p orbitals are drawn.



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

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



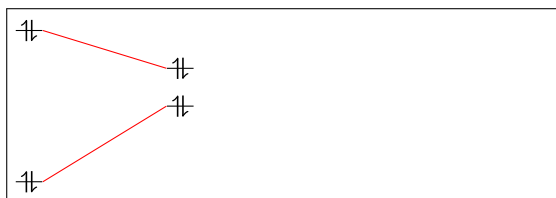
```
1 \begin{MOfdiagram}
2 \atom{left} {1s=0}
3 \atom{right}{1s=0}
4 \molecule {1sMO=1}
5 \AO(1cm){s}{2}
6 \AO(3cm){s}{2}
7 \AO(5cm){s}{2}
8 \end{MOfdiagram}
```

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):



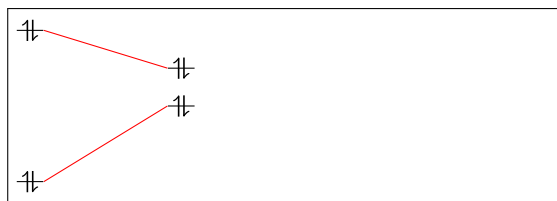
```
1 \begin{MOfdiagram}
2 \atom{left} {2p=0}
3 \atom{right}{2p=0}
4 % above the left atom:
5 \AO(1cm) {s}{.5}
6 \AO(1cm-20pt){s}{1;up}
7 \AO(1cm-40pt){s}{1.5;down}
8 % above the right atom:
9 \AO(5cm) {s}{.5}
10 \AO(5cm+20pt){s}{1;up}
11 \AO(5cm+40pt){s}{1.5;down}
12 \end{MOfdiagram}
```

The AO created with \AO also can be connected. For this you can use the TikZ command \draw, of course. You can use the predefined node names ...



```
1 \begin{MOfdiagram}
2 \AO{s}{0} \AO(2cm){s}{1}
3 \AO{s}{2} \AO(2cm){s}{1.5}
4 \draw[red] (AO1.0) -- (AO
5 2.180) (AO3.0) -- (AO
6 4.180);
7 \end{MOfdiagram}
```

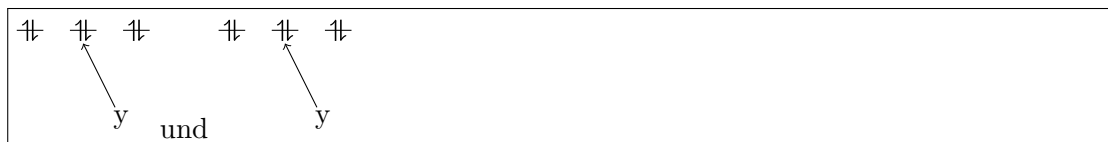
... or use own node names



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

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 a **x**, **y** or a **z** if you specify your own name, too.

```
1 \begin{MObdiagram}
2 \AO{p}{0}
3 \draw[<-,shorten >=5pt] (AO1y.-90) -- ++ (.5,-1) node {y};
4 \end{MObdiagram}
5 und
6 \begin{MObdiagram}
7 \AO[A]{p}{0}
8 \draw[<-,shorten >=5pt] (Ay.-90) -- ++ (.5,-1) node {y};
9 \end{MObdiagram}
```

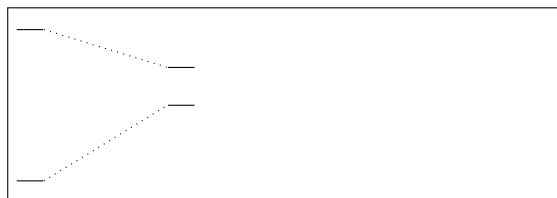


However, if you want the lines to be drawn in the same style as the ones created by **\molecule**⁶, you should use the command **\connect**.

\connect{<AO-connect>}

- **<AO-connect>** (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 **&**:



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

⁶which 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 *TikZ* way:



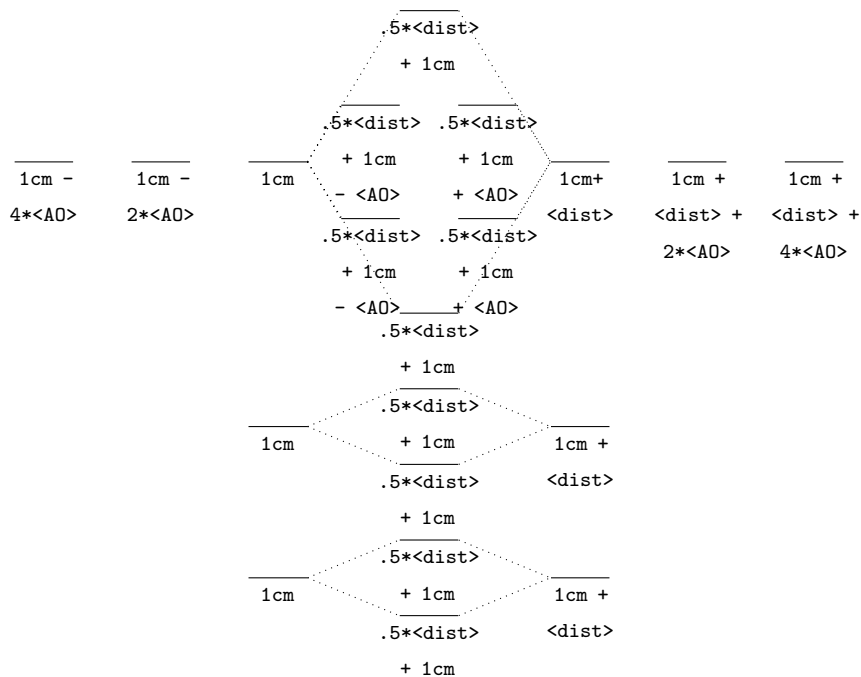
```

1 \begin{tikzpicture}
2   \draw (0,0) node (a) {a} ++
      (1,0) node (b) {b}
3     ++ (0,1) node (c) {c}
      ++ (-1,0) node (d)
          {d} ;
4   \connect{ a.90 & d.-90, c
      .180 & d.0 }
5 \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.



3.6 Default Values

NEW 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 11); It needs a value for `<energy>`, though.

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

Compare these examples:



```

1 \begin{MOdiagram}
2 \atom{left} { 1s={0;pair} }
3 \atom{right}{ 1s }
4 \end{MOdiagram}
5
6 \hrulefill
7
8 \begin{MOdiagram}
9 \atom{left}{ 1s=1 }
10 \atom{right}{ 1s= }
11 \end{MOdiagram}

```

4 Customization

The 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 between 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 `TikZ` 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 `TikZ` style of the captions, section 4.1.7.
- `names-style-add=<tikz>` change the `TikZ` 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 `TikZ` 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're set locally and only change that environment.

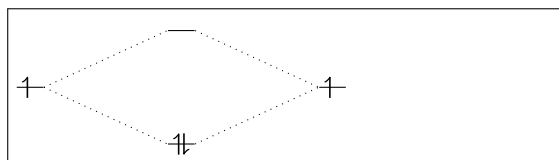
```
1 \begin{MOdiagram}[<key = value>]
2 ...
3 \end{MOdiagram}
```

4.1.1 Option style

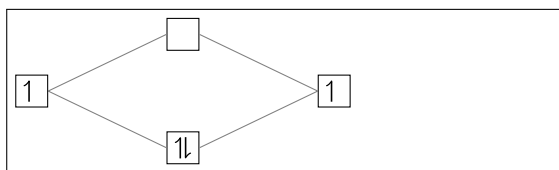
There are five different styles, which can be chosen.

- `style=plain` \uparrow (default)
- `style=square` $\boxed{\uparrow}$
- `style=circle` $\textcircled{\uparrow}$
- `style=round` $\boxed{\uparrow}$
- `style=fancy` $\boxed{\uparrow}$

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



```
1 % use package 'mhchem'
2 \begin{MOdiagram}[style=plain
  ]% default
3 \atom[H]{left} { 1s = {;up}
  }
4 \atom[H]{right}{ 1s = {;up}
  }
5 \molecule[\ce{H2}]{ 1sMO =
  {.75;pair} }
6 \end{MOdiagram}
```

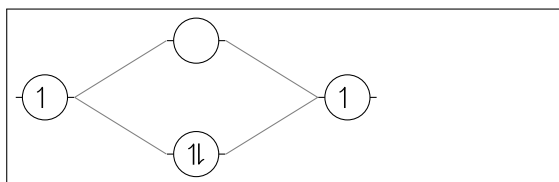



```

1 % use package 'mhchem'
2 \begin{MObdiagram}[style=
  square]
3 \atom[H]{left} { 1s = {};up}
  }
4 \atom[H]{right}{ 1s = {};up}
  }
5 \molecule[\ce{H2}]{ 1sMO =
  {.75;pair} }
6 \end{MObdiagram}

```

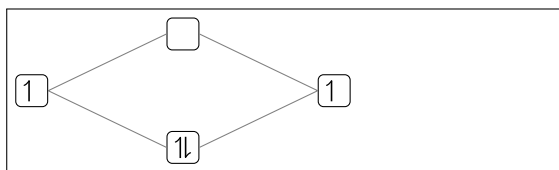
NEW



```

1 % use package 'mhchem'
2 \begin{MObdiagram}[style=
  circle]
3 \atom[H]{left} { 1s = {};up}
  }
4 \atom[H]{right}{ 1s = {};up}
  }
5 \molecule[\ce{H2}]{ 1sMO =
  {.75;pair} }
6 \end{MObdiagram}

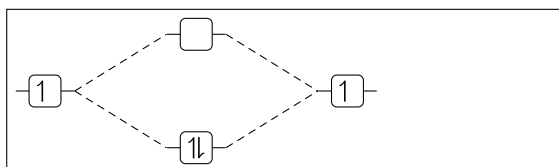
```



```

1 % use package 'mhchem'
2 \begin{MObdiagram}[style=round
  ]
3 \atom[H]{left} { 1s = {};up}
  }
4 \atom[H]{right}{ 1s = {};up}
  }
5 \molecule[\ce{H2}]{ 1sMO =
  {.75;pair} }
6 \end{MObdiagram}

```



```

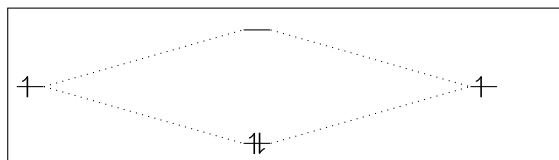
1 % use package 'mhchem'
2 \begin{MObdiagram}[style=fancy
  ]
3 \atom[H]{left} { 1s = {};up}
  }
4 \atom[H]{right}{ 1s = {};up}
  }
5 \molecule[\ce{H2}]{ 1sMO =
  {.75;pair} }
6 \end{MObdiagram}

```

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

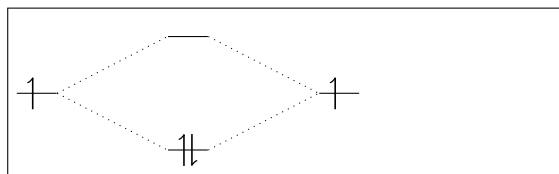
position of the right atom is changed to $1\text{cm} + \langle \text{dim} \rangle$ and the position of the molecule is changed to $0.5 \cdot (1\text{cm} + \langle \text{dim} \rangle)$, also see page 12 and section 3.5.



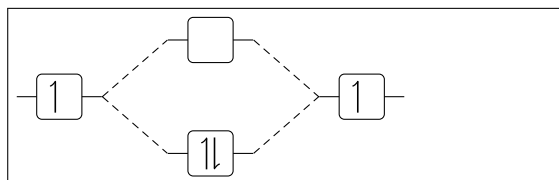
```
1 % use package 'mhchem'
2 \begin{MOfdiagram}[distance=6
  cm]
3 \atom[H]{left} { 1s = {;up}
  }
4 \atom[H]{right}{ 1s = {;up}
  }
5 \molecule[\ce{H2}]{ 1sMO =
  {.75;pair} }
6 \end{MOfdiagram}
```

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. Its default value is 10 pt.



```
1 % use package 'mhchem'
2 \begin{MOfdiagram}[AO-width=15
  pt]
3 \atom[H]{left} { 1s = {;up}
  }
4 \atom[H]{right}{ 1s = {;up}
  }
5 \molecule[\ce{H2}]{ 1sMO =
  {.75;pair} }
6 \end{MOfdiagram}
```

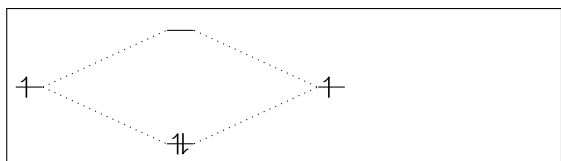


```
1 % use package 'mhchem'
2 \begin{MOfdiagram}[style=fancy
  ,AO-width=15pt]
3 \atom[H]{left} { 1s = {;up}
  }
4 \atom[H]{right}{ 1s = {;up}
  }
5 \molecule[\ce{H2}]{ 1sMO =
  {.75;pair} }
6 \end{MOfdiagram}
```

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

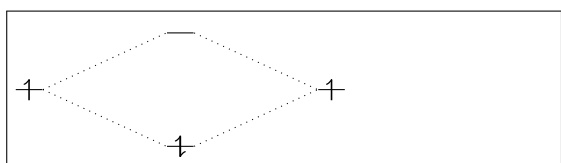
NEW These three options change the horizontal positions of the arrows representing the electrons in a AO/MO. The option `el-sep=<num>` needs a value between 0 and 1. 0 means *no* distance between the arrows and 1 *full* distance (with respect to the length `AO-width`, see section 4.1.3).



```

1 % use package 'mhchem'
2 \begin{MoleculeDiagram}[el-sep=.2]%
   default
3 \atom[H]{left} { 1s = {};up}
   }
4 \atom[H]{right}{ 1s = {};up}
   }
5 \molecule[\ce{H2}]{ 1sMO =
   {.75;pair} }
6 \end{MoleculeDiagram}

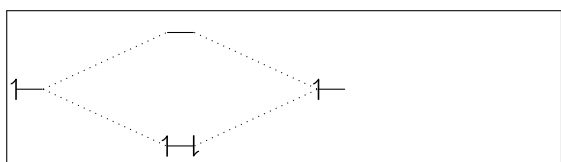
```



```

1 % use package 'mhchem'
2 \begin{MoleculeDiagram}[el-sep=0]
3 \atom[H]{left} { 1s = {};up}
   }
4 \atom[H]{right}{ 1s = {};up}
   }
5 \molecule[\ce{H2}]{ 1sMO =
   {.75;pair} }
6 \end{MoleculeDiagram}

```

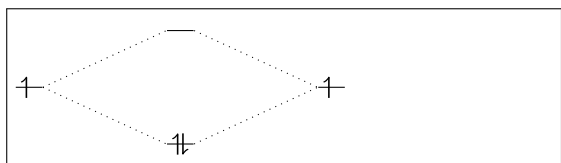


```

1 % use package 'mhchem'
2 \begin{MoleculeDiagram}[el-sep=1]
3 \atom[H]{left} { 1s = {};up}
   }
4 \atom[H]{right}{ 1s = {};up}
   }
5 \molecule[\ce{H2}]{ 1sMO =
   {.75;pair} }
6 \end{MoleculeDiagram}

```

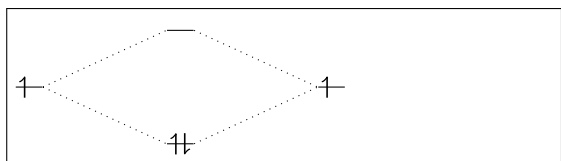
The options `up-el-pos=<num>` and `down-el-pos=<num>` can be used alternatively to place the spin-up and spin-down electron, respectively. Again they need values between 0 and 1. This time 0 means *on the left* and 1 means *on the right*



```

1 % use package 'mhchem'
2 \begin{MoleculeDiagram}[up-el-pos
   =.4,down-el-pos=.6]%
   default
3 \atom[H]{left} { 1s = {};up}
   }
4 \atom[H]{right}{ 1s = {};up}
   }
5 \molecule[\ce{H2}]{ 1sMO =
   {.75;pair} }
6 \end{MoleculeDiagram}

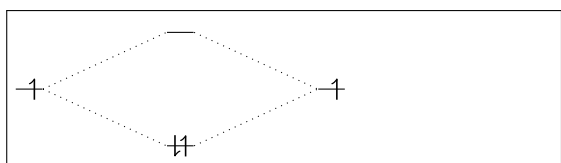
```



```

1 % use package 'mhchem'
2 \begin{MOfdiagram}[up-el-pos
  =.333,down-el-pos=.667]
3 \atom[H]{left} { 1s = {};up}
  }
4 \atom[H]{right}{ 1s = {};up}
  }
5 \molecule[\ce{H2}]{ 1sMO =
  {.75;pair} }
6 \end{MOfdiagram}

```



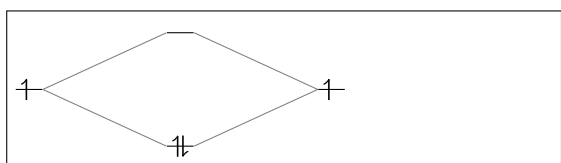
```

1 % use package 'mhchem'
2 \begin{MOfdiagram}[up-el-pos
  =.7,down-el-pos=.3]
3 \atom[H]{left} { 1s = {};up}
  }
4 \atom[H]{right}{ 1s = {};up}
  }
5 \molecule[\ce{H2}]{ 1sMO =
  {.75;pair} }
6 \end{MOfdiagram}

```

4.1.5 Option lines

The option `lines` can be used to modify the `TikZ` style of the connecting lines:



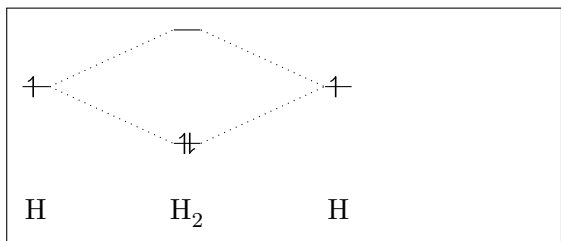
```

1 % use package 'mhchem'
2 \begin{MOfdiagram}[lines={gray
  ,thin}]
3 \atom[H]{left} { 1s = {};up}
  }
4 \atom[H]{right}{ 1s = {};up}
  }
5 \molecule[\ce{H2}]{ 1sMO =
  {.75;pair} }
6 \end{MOfdiagram}

```

4.1.6 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`.



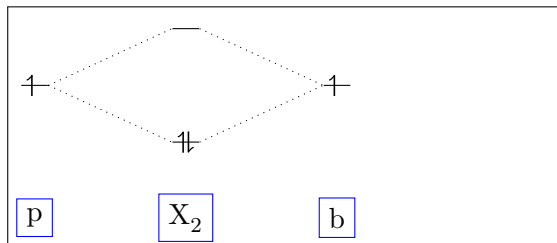
```

1 % use package 'mhchem'
2 \begin{MOfdiagram}[names]
3 \atom[H]{left} { 1s = {};up}
  }
4 \atom[H]{right}{ 1s = {};up}
  }
5 \molecule[\ce{H2}]{ 1sMO =
  {.75;pair} }
6 \end{MOfdiagram}

```

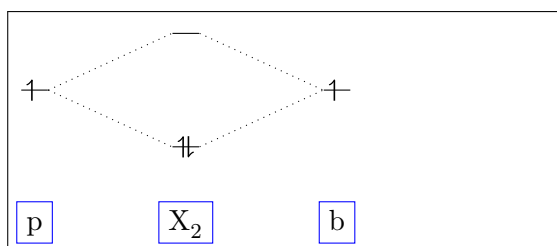
4.1.7 Optionen `names-style` und `names-style-add`

NEW 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.



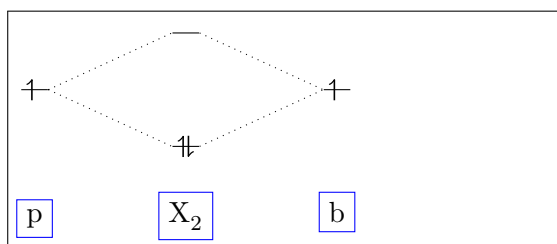
```
1 % use package 'mhchem'
2 \begin{MObdiagram}[names,names
  -style={draw=blue}]
3 \atom[p]{left} { 1s = {};up}
  }
4 \atom[b]{right}{ 1s = {};up}
  }
5 \molecule[\ce{X2}]{ 1sMO =
  {.75;pair} }
6 \end{MObdiagram}
```

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



```
1 % use package 'mhchem'
2 \begin{MObdiagram}[names,names
  -style={text height=1.5ex,
    text depth=.25ex, draw=
    blue}]
3 \atom[p]{left} { 1s = {};up}
  }
4 \atom[b]{right}{ 1s = {};up}
  }
5 \molecule[\ce{X2}]{ 1sMO =
  {.75;pair} }
6 \end{MObdiagram}
```

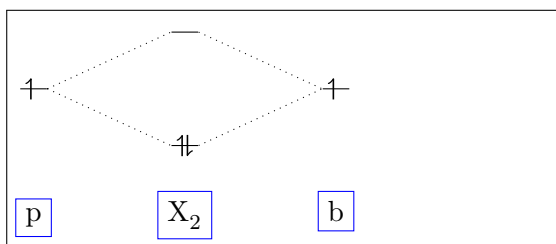
..., add the `anchor` again ...



```
1 % use package 'mhchem'
2 \begin{MObdiagram}[names,names
  -style={anchor=base, draw=
    blue}]
3 \atom[p]{left} { 1s = {};up}
  }
4 \atom[b]{right}{ 1s = {};up}
  }
5 \molecule[\ce{X2}]{ 1sMO =
  {.75;pair} }
6 \end{MObdiagram}
```

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

⁷Please see "TikZ und PGF – Manual for Version 2.10" p. 183 section 16.4.4 (pgfmanual.pdf) for the meaning



```

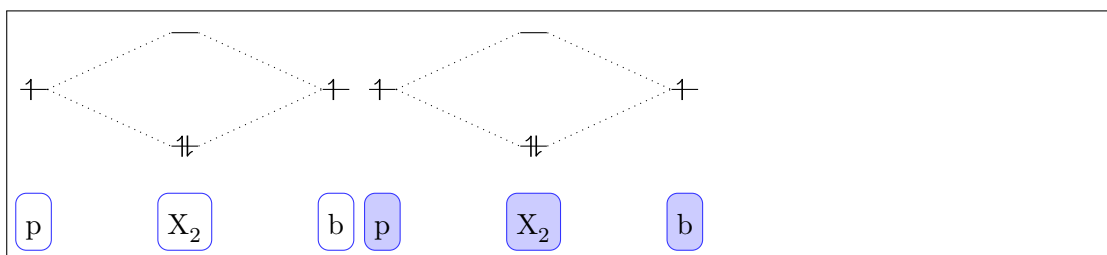
1 % use package 'mhchem'
2 \begin{MOfdiagram}[names,names
  -style-add={draw=blue}]
3 \atom[p]{left} { 1s = {};up}
  }
4 \atom[b]{right}{ 1s = {};up}
  }
5 \molecule[\ce{X2}]{ 1sMO =
  {.75;pair} }
6 \end{MOfdiagram}

```

```

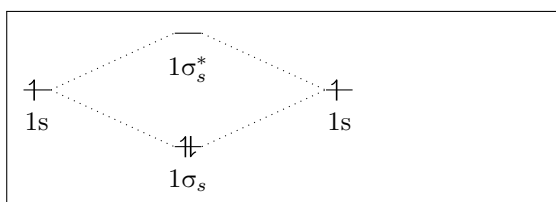
1 \MOsetup{names,names-style={text height=2.5ex,text depth=.5ex,
  draw=blue!80,rounded corners}}
2 \begin{MOfdiagram}
3 \atom[p]{left} { 1s = {};up} }
4 \atom[b]{right}{ 1s = {};up} }
5 \molecule[\ce{X2}]{ 1sMO = {.75;pair} }
6 \end{MOfdiagram}
7 \begin{MOfdiagram}[names-style-add={fill=blue!20}]
8 \atom[p]{left} { 1s = {};up} }
9 \atom[b]{right}{ 1s = {};up} }
10 \molecule[\ce{X2}]{ 1sMO = {.75;pair} }
11 \end{MOfdiagram}

```



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.



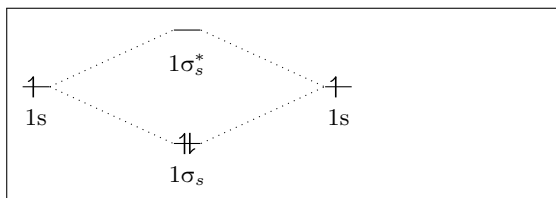
```

1 % use package 'mhchem'
2 \begin{MOfdiagram}[labels]
3 \atom[H]{left} { 1s = {};up}
  }
4 \atom[H]{right}{ 1s = {};up}
  }
5 \molecule[\ce{H2}]{ 1sMO =
  {.75;pair} }
6 \end{MOfdiagram}

```

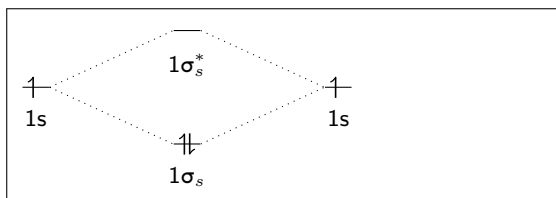
4.1.9 Option labels-fs

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



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

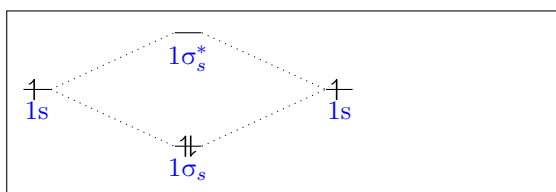
This also allows you to change the font style or font shape of the labels.



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

4.1.10 Option labels-style

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

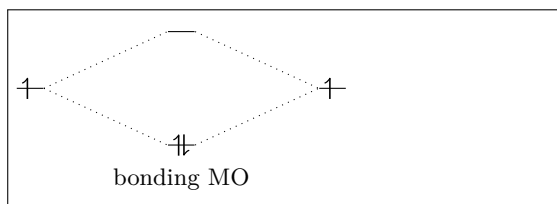


```
1 % use package 'mhchem'
2 \begin{MOfdiagram}[labels,
   labels-style={blue,yshift
   =4pt}]
3 \atom[H]{left} { 1s = {};up}
4 \atom[H]{right}{ 1s = {};up}
5 \molecule[\ce{H2}]{ 1sMO =
   {.75;pair} }
6 \end{MOfdiagram}
```

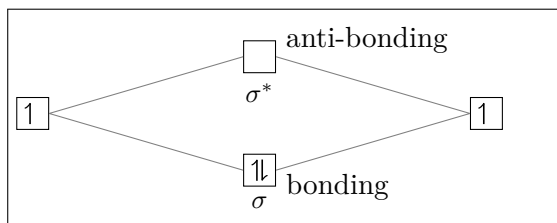
4.2 `\atom` and `\molecule` Specific Customizations

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.

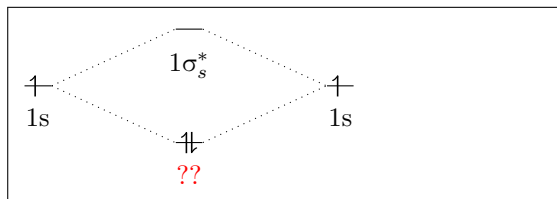


```
1 % use package 'mhchem'
2 \begin{MOdiagram}[labels=fs=\footnotesize]
3 \atom[H]{left} { 1s = {};up}
4 \atom[H]{right}{ 1s = {};up}
5 \molecule[\ce{H2}]{
6   1sMO = {.75;pair},
7   label = { 1sigma = {
8     bonding MO} }
9 }
10 \end{MOdiagram}
```



```
1 \begin{MOdiagram}[style=square,distance=6cm]
2 \atom{left} { 1s = {};up} }
3 \atom{right}{ 1s = {};up} }
4 \molecule{
5   1sMO = {.75;pair} ,
6   label = {
7     1sigma = {\sigma},
8     1sigma* = {\sigma^*}
9   }
10 }
11 \node[right] at (1sigma.-45)
12   {bonding};
13 \node[right] at (1sigma*.45)
14   {anti-bonding};
15 \end{MOdiagram}
```

If the key is used together with the `labels` option (page 22), single labels are overwritten:



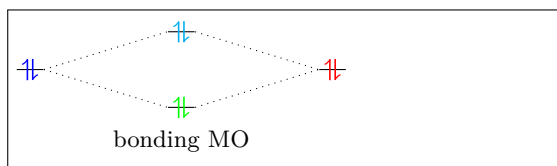
```

1 % use package 'mhchem'
2 \begin{MOfdiagram}[labels]
3 \atom[H]{left} { 1s = {;up}
4   }
5 \atom[H]{right}{ 1s = {;up}
6   }
7 \molecule[\ce{H2}]{
8   1sMO = {.75;pair},
9   label = { 1sigma = \
10     textcolor{red}{??} }
11 }
12 \end{MOfdiagram}

```

4.2.2 The color Key

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



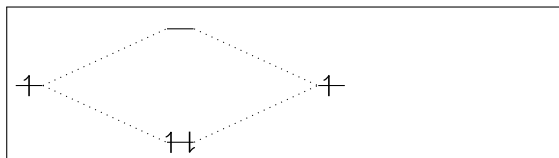
```

1 % use package 'mhchem'
2 \begin{MOfdiagram}[labels-fs=\
3   footnotesize]
4 \atom[H]{left}{
5   1s, color = { 1sleft =
6     blue }
7 }
8 \atom[H]{right}{
9   1s, color = { 1sright =
10     red }
11 }
12 \molecule[\ce{H2}]{
13   1sMO,
14   label = { 1sigma = {
15     bonding MO} },
16   color = { 1sigma = green,
17     1sigma* = cyan }
18 }
19 \end{MOfdiagram}

```

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

NEW 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.



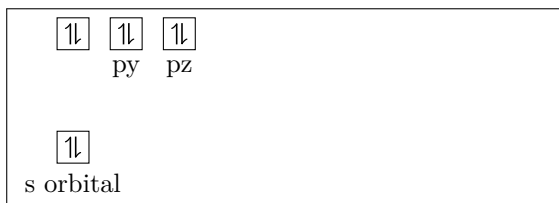
```
1 % use package 'mhchem'
2 \begin{MObdiagram}
3 \atom[H]{left}{
4   1s          = {;up},
5   up-el-pos = { 1sleft=.5 }
6 }
7 \atom[H]{right}{ 1s = {;up}
8 }
9 \molecule[\ce{H2}]{
10  1sMO          = {.75;pair} ,
11  up-el-pos     = { 1sigma=.15
12                  } ,
13  down-el-pos  = { 1sigma=.85
14                  }
15 }
16 \end{MObdiagram}
```

4.3 \AO Specific Customizations

NEW 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:



```
1 \begin{MObdiagram}[style=
2   square]
3 \AO{s}[label={s orbital}]{0}
4 \AO{p}[label[y]=py,label[z]=
5   pz]{1.5}
6 \end{MObdiagram}
```

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:



```
1 \begin{MObdiagram}[style=
2   square]
3 \AO{s}[color=red]{0}
4 \AO{p}[color[y]=green,color[
5   z]=cyan]{1.5}
6 \end{MObdiagram}
```

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:



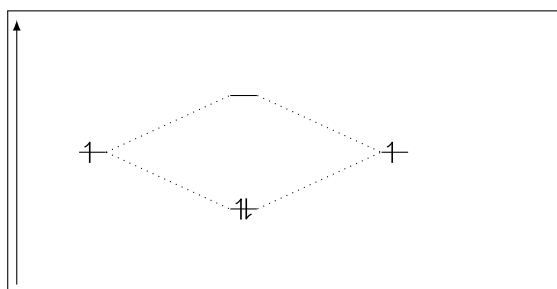
```
1 \begin{MOdiagram}[style=
   square]
2 \AO{s}[up-el-pos=.15]{0}
3 \AO{p}[up-el-pos[y]=.15,down
   -el-pos[z]=.15]{1.5}
4 \end{MOdiagram}
```

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>]`

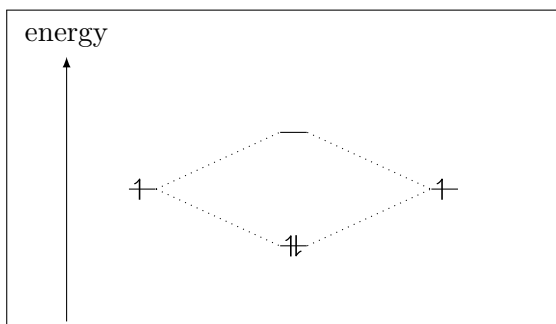
- `<key = val>` (o) ey/value pairs to modify the axis



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

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

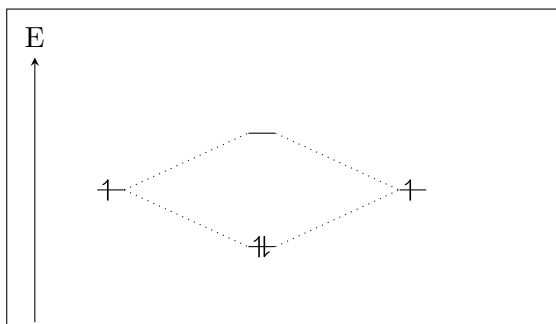
- `title=<title>` axis label (default: `energy`).
- `head=<tikz-arrow-head>` arrow head; you can use the arrow heads specified in the *TikZ* library `arrows`⁸ (pgfmanual v2.10 pages 256ff.) (default: `>`).



```

1 \begin{MOfdiagram}
2 \atom{left} { 1s = {;up} }
3 \atom{right}{ 1s = {;up} }
4 \molecule{ 1sMO = {.75;pair}
5 }
6 \EnergyAxis [title]
7 \end{MOfdiagram}

```



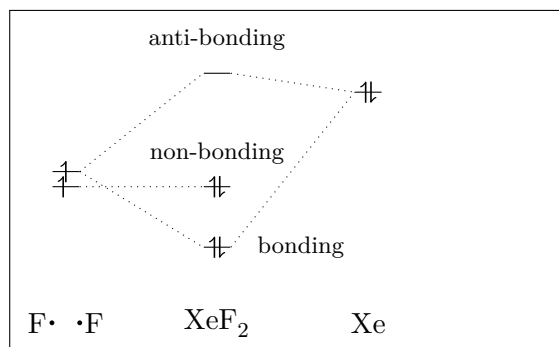
```

1 \begin{MOfdiagram}
2 \atom{left} { 1s = {;up} }
3 \atom{right}{ 1s = {;up} }
4 \molecule{ 1sMO = {.75;pair}
5 }
6 \EnergyAxis [title=E,head=
7 stealth]
8 \end{MOfdiagram}

```

5 Examples

The example from the beginning of section 3.4.



```

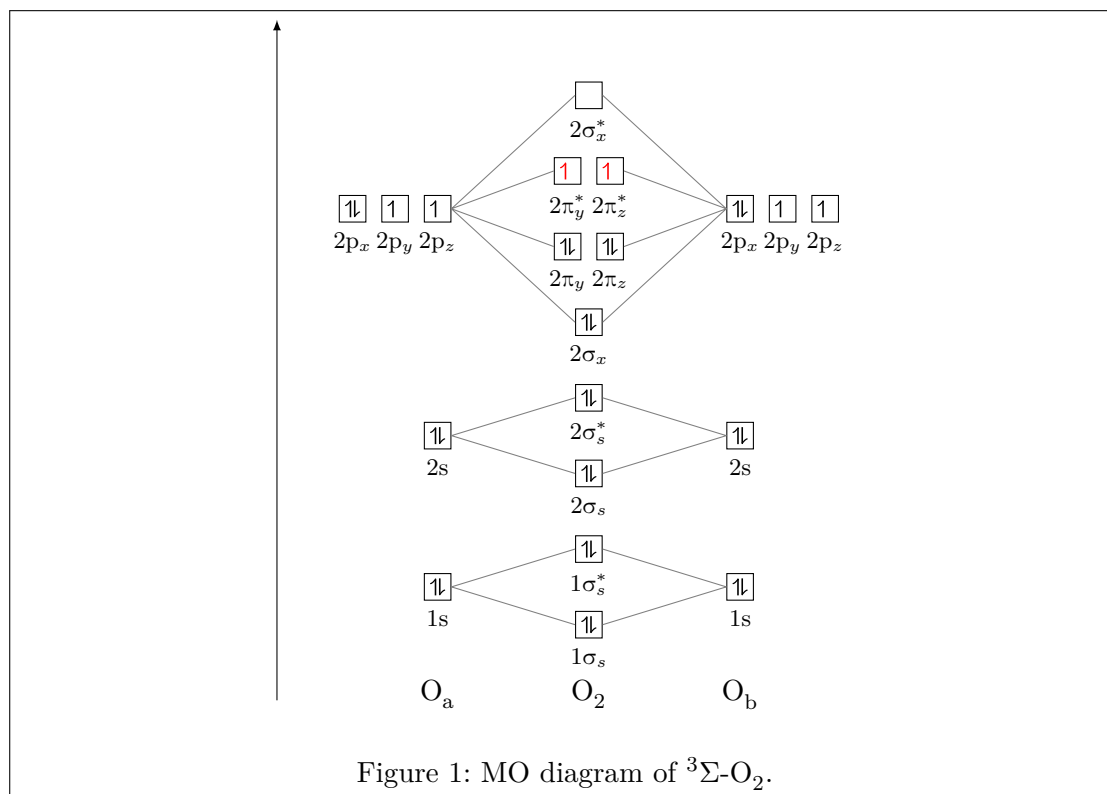
1 % use packages 'mhchem' and '
  chemfig'
2 \begin{MOfdiagram}[names,names
  -style={}]
3 \atom[\lewis{0.,F}\hspace*{5
  mm}\lewis{4.,F}]{left}{1s
  =.2;up,up-el-pos={1sleft
  =.5}}
4 \atom[Xe]{right}{1s=1.25;
  pair}
5 \molecule[\ce{XeF2}]{1sMO
  ={1/.25;pair}}
6 \AO(1cm){s}{0;up}
7 \AO(3cm){s}{0;pair}
8 \connect{ AO1 & AO2 }
9 \node[right,xshift=4mm] at
  (1sigma) {\footnotesize
  bonding};
10 \node[above] at (AO2.90) {\
  footnotesize non-bonding
  };
11 \node[above] at (1sigma*.90)
  {\footnotesize anti-
  bonding};
12 \end{MOfdiagram}

```

```

1 % use packages 'mhchem' (and 'textgreek' loaded by 'MOdiagram')
2 \begin{figure}
3   \centering
4   \begin{MOdiagram}[style=square,labels,names,AO-width=8pt,labels
5     -fs=\footnotesize]
6     \atom[\ce{O_a}]{left}{
7       1s, 2s, 2p = {};pair,up,up}
8     }
9     \atom[\ce{O_b}]{right}{
10      1s, 2s, 2p = {};pair,up,up}
11    }
12    \molecule[\ce{O2}]{
13      1sMO, 2sMO, 2pMO = {};pair,pair,pair,up,up},
14      color = { 2piy*=red, 2piz*=red }
15    }
16    \EnergyAxis
17  \end{MOdiagram}
18  \caption{MO diagram of  ${}^3\Sigma-\text{O}_2$ .}
19 \end{figure}

```



```

1 % use package 'chemfig'
2 \begin{figure}
3 \centering\MOsetup{style = fancy, distance = 7cm, AO-width = 15
4 pt, labels}
5 \begin{MOdiagram}
6 \atom[N]{left}{
7   2p = {0;up,up,up}
8 }
9 \atom[O]{right}{
10   2p = {2;pair,up,up}
11 }
12 \molecule[NO]{
13   2pMO = {1.8,.4;pair,pair,pair,up},
14   color = { 2piy*=red }
15 }
16 \EnergyAxis
17 \end{MOdiagram}
18 \caption{Part of the MO diagram of \protect\Lewis{4.,NO}..}
19 \end{figure}

```

