# ENDIAGRAM

v0.1d 2014/06/28

Easy creation of potential energy curve diagrams

Clemens Niederberger

https://bitbucket.org/cgnieder/endiagram/

contact@mychemistry.eu

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# 1 Licence and Requirements

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

ENDIAGRAM needs the l3kernel [Tea13] and the package xparse. xparse is part of the l3packages [Tea] bundle. ENDIAGRAM also needs Ti*k*Z [Tan10] and siunitx [Wri13].

Basic knowledge of Ti*k*Z/pgf is recommended.

# 2 Caveat

This package is in an experimental state. There is lots of code to clean up and there are many loose ends to be tied together until I'll be satisfied to publish this package as stable. However, as the unofficial release on my blog has gotten quite some interest[1] I decided to publish this experimental version on the Comprehensive TeX Archive Network nonetheless.

If you detect any bugs – and I guess you will – please write me a short email with a minimal working example (MWE) showing the undesired behaviour or report on issue on `https://www.bitbucket.org/cgnieder/endiagram`.

# 3 Setup

There are two kinds of options: choice options where you can choose one of the values separated with `|`; an underlined value is a default value that is used, if no value is given. The others need a value of a certain type like a number (⟨*num*⟩), arbitrary input (⟨*text*⟩), Ti*k*Z options (⟨*tikz*⟩) *etc.*

As a rule commands are only defined inside the `endiagram` environment.

Options can also be set up with this command:

`\ENsetup[`⟨*module*⟩`]{`⟨*options*⟩`}`

The setup command.

```
\ENsetup{option1 = value1, option2 = value2}
\ENsetup{module/option = value}
\ENsetup[module]{option = value}
```

Options that belong to a module are specific to a command. The command `\command` they belong to can *only* have the options marked with `command` in his argument `[`⟨*options*⟩`]`.

All other options can also be set globally as package options. These are options which do *not* belong to a module like for example the `draft` = `{`⟨*o*⟩`}`ption (see page 11):

1. ≥ 400 downloads

```
\usepackage[draft]{endiagram}
```

## 4 The Curve – \ENcurve

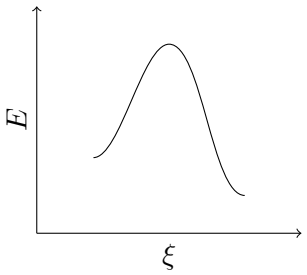
The potential energy curves are drawn inside the `endiagram` environment using the command `\ENcurve`.

`\begin{endiagram}[`⟨*options*⟩`]`
The basic environment for the potential energy curves

`\ENcurve[`⟨*options*⟩`]{`⟨*level1*⟩`,`⟨*level2*⟩`,`⟨*level3*⟩`}`
The basic command for drawing the actual curve.

The command needs a comma separated list of relative energy levels. `\ENcurve{1,4,0}` means the maximum is four times higher above the end level than the starting level.

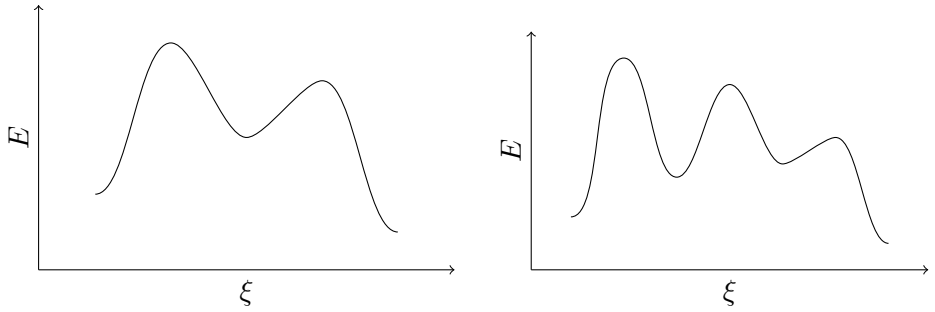
```
\begin{endiagram}
  \ENcurve{1,4,0}
\end{endiagram}
```




`\ENcurve` can read any number of values but needs *at least three*. Less values will cause an error.

```
\begin{endiagram}
  \ENcurve{1,5,2.5,4,0}
\end{endiagram}
\quad
\begin{endiagram}[scale=.7]
  \ENcurve{1,7,2.5,6,3,4,0}
\end{endiagram}
```

---




## 4.1 Properties

### 4.1.1 Scaling

Values given to \ENcurve are multiples of ENDIAGRAM's standard unit (SU). As a default it is set to 0.5 cm but can be changed using an option. There are other ways to influence the size of the diagram, too.

unit = {⟨*length*⟩} Default: .5cm

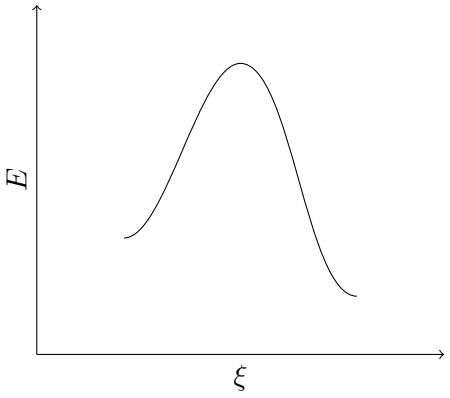
The standard unit for \ENcurve and some other commands. This document refers to it with SU.

scale = {⟨*factor*⟩} Default: 1

A scaling factor that allows scaling the diagram.

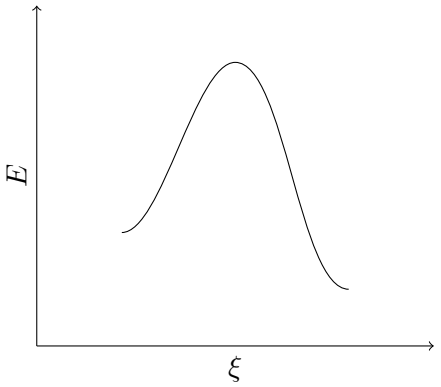
A changed SU:

```
\begin{endiagram}[unit=2em]
  \ENcurve{1,4,0}
\end{endiagram}
```




Scaled by the factor 1.5:

```
\begin{endiagram}[scale=1.5]
  \ENcurve{1,4,0}
\end{endiagram}
```




### 4.1.2 Influencing the position relative to the axes

The `offset` options control the length and position of the horizontal axis relative to the curve.

`offset` = {⟨*num*⟩} Default: `0`

⟨*num*⟩ is a multiple of the SU (see page 4).

`r-offset` = {⟨*num*⟩} Default: `0`

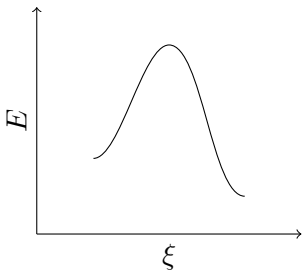
⟨*num*⟩ is a multiple of the SU.

`l-offset` = {⟨*num*⟩} Default: `0`

⟨*num*⟩ is a multiple of the SU.

The default behaviour for comparison:

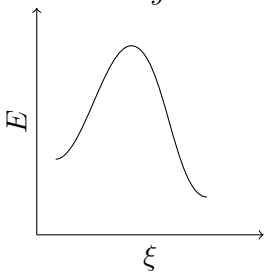
```
\begin{endiagram}
  \ENcurve{1,4,0}
\end{endiagram}
```




`l-offset` controls the distance of the start of the $x$ axis to the start of the curve:

```
closer to the $y$ axis:\par
\begin{endiagram}[l-offset=-1]
  \ENcurve{1,4,0}
\end{endiagram}
```

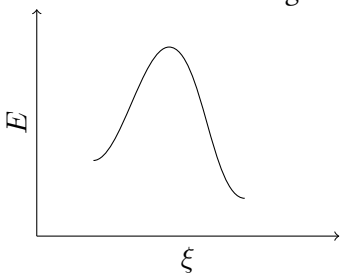
closer to the $y$ axis:



r-offset controls the "protruding" of the $x$ axis after the curve:

```
$x$ axis extended to the right:\par
\begin{endiagram}[r-offset=1]
  \ENcurve{1,4,0}
\end{endiagram}
```

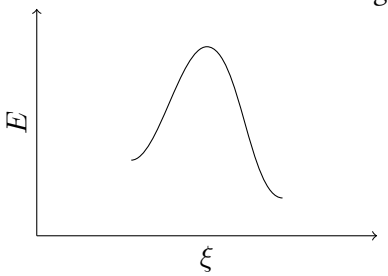
$x$ axis extended to the right:




offset changes both values equally:

```
$x$ extended to the left and the right
  :\par
\begin{endiagram}[offset=1]
  \ENcurve{1,4,0}
\end{endiagram}
```

$x$ extended to the left and the right:



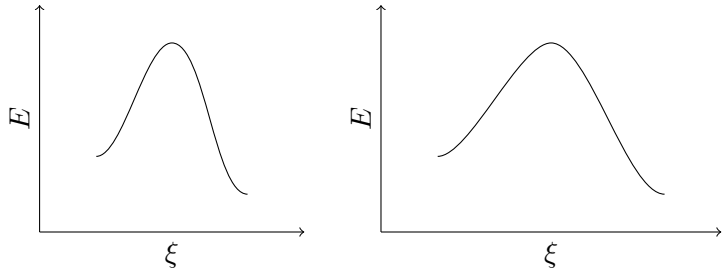

### 4.1.3 Increment between the levels

With the option step the default increment between the levels can be changed:

ENcurve » step = {⟨num⟩} Default: 2

⟨num⟩ is a multiple of the su (see page 4).

```
\begin{endiagram}
  \ENcurve{1,4,0}
\end{endiagram}
\quad
\begin{endiagram}
  \ENcurve[step=3]{1,4,0}
\end{endiagram}
```

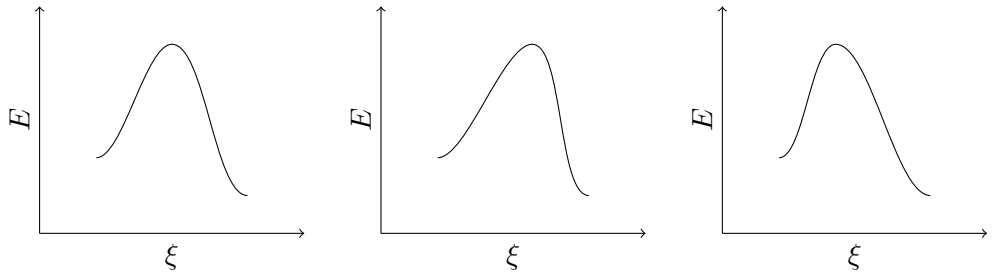



Sometimes a certain level should be shifted against the others. This is possible using an optional argument to the value of that level:

`\ENcurve{`⟨*level*⟩`[`⟨*offset*⟩`],...}`

⟨*offset*⟩ is a multiple of the SU (see page 4) and is set to `0` as default. The level will be shifted to the right (positive values) or left (negative values).

```
\begin{endiagram}
  \ENcurve{1,4,0}
\end{endiagram}
\quad
\begin{endiagram}
  \ENcurve{1,4[.5],0}
\end{endiagram}
\quad
\begin{endiagram}
  \ENcurve{1,4[-.5],0}
\end{endiagram}
```



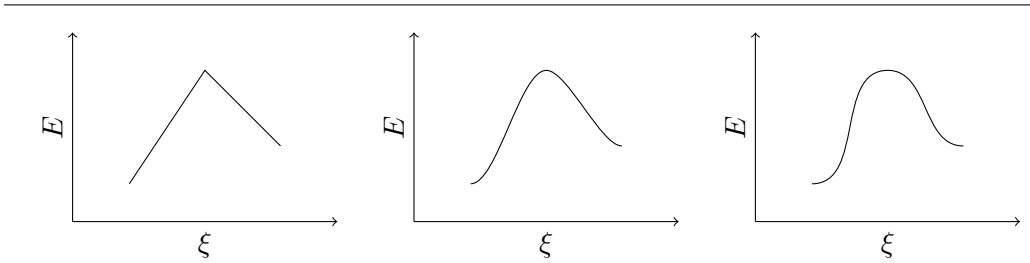

### 4.1.4 The shape

The option `looseness` changes the shape of the curve:

`ENcurve` » `looseness` = `{`⟨*value*⟩`}` Default: `.5`

should be a number between `0` and `1`.

```
\begin{endiagram}
  \ENcurve[looseness=0]{0,3,1}
\end{endiagram}
\quad
\begin{endiagram}
  \ENcurve{0,3,1}% corresponds looseness=.5
\end{endiagram}
\quad
\begin{endiagram}
  \ENcurve[looseness=1]{0,3,1}
\end{endiagram}
```



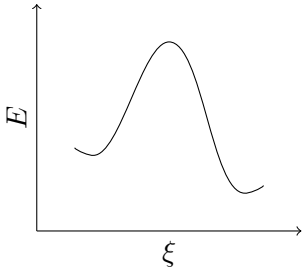

### 4.1.5 Ending minima

Sometimes potential energy curves are drawn with local minima at the start and the end of the cuve. The option `minima` en- or disables them:

`ENcurve` » `minima` = `true`|`false` Default: `false`

Draw local minima at the ends of the curve.

```
\begin{endiagram}
  \ENcurve[minima]{1,4,0}
\end{endiagram}
```



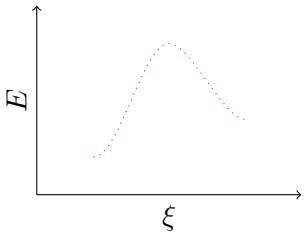

### 4.1.6 TikZ style

The style of the curve can be changed using TikZ options:

`ENcurve` » `tikz` = {⟨*tikz*⟩} (initially empty)

Valid are options that can be used with `\draw`.

```
\begin{endiagram}
  \ENcurve[tikz={red,dotted}]{0,3,1}
\end{endiagram}
```




## 4.2 The Axes

There are also possibilities to customize the axes.

`axes` = `xy|y|y-l|y-r|x|all|false` Default: `xy`
Number and type of axes.

`x-axis` = {⟨*tikz*⟩} (initially empty)
Ti*k*Z options to the $x$ axis.

`y-axis` = {⟨*tikz*⟩} (initially empty)
Ti*k*Z options to the $y$ axis.

`x-label` = `below|right` Default: `below`
Position of the $x$ axis label.

`y-label` = `above|left` Default: `left`
Position of the $y$ axis label.

`x-label-pos` = {⟨*value*⟩} Default: `.5`
Position of the $x$ axis label when `x-label` = `{below}` is set.

`y-label-pos` = {⟨*value*⟩} Default: `.5`
Position of the $y$ axis label when `y-label` = `{left}` is set.

`x-label-offset` = {⟨*length*⟩} Default: `0pt`
Distance between label and $x$ axis.

`y-label-offset` = {⟨*length*⟩} Default: `0pt`
Distance between label and $y$ axis.

`x-label-angle` = {⟨*angle*⟩} Default: `0`
Angle which rotates the $x$ axis label counter clockwise.

`y-label-angle` = {⟨*angle*⟩} Default: `0`
Angle which rotates the $y$ axis label counter clockwise.

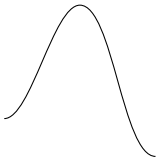
`x-label-text` = {⟨*text*⟩} Default: `$\xi$`
$x$ axis label.

`y-label-text` = {⟨*text*⟩} Default: `$E$`

$y$ axis label.

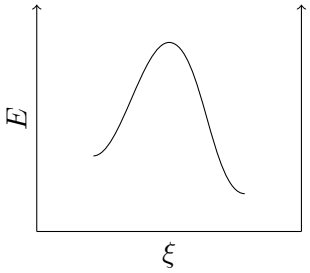
No axes:

```
\begin{endiagram}[axes=false]
  \ENcurve{1,4,0}
\end{endiagram}
```



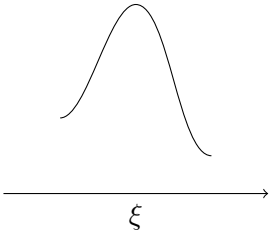
All axes:

```
\begin{endiagram}[axes=all]
  \ENcurve{1,4,0}
\end{endiagram}
```



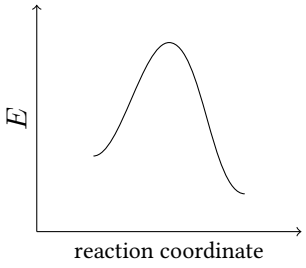

Only the $x$ axis:

```
\begin{endiagram}[axes=x]
  \ENcurve{1,4,0}
\end{endiagram}
```



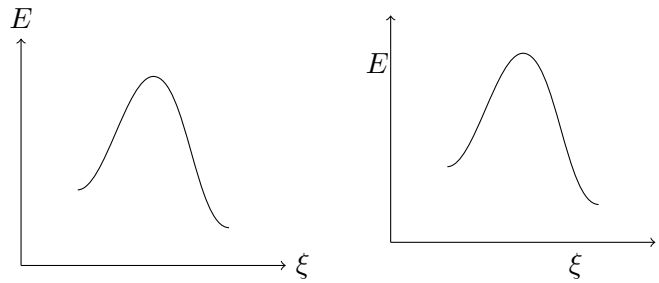

Changed labels:

```
\begin{endiagram}[x-label-text=\
  footnotesize reaction coordinate]
  \ENcurve{1,4,0}
\end{endiagram}
```



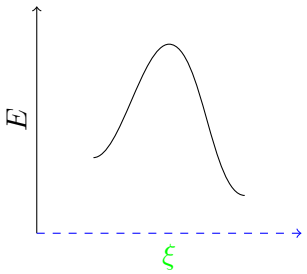

Different positions of the labels:

```
\begin{endiagram}[
   x-label=right,
   y-label=above]
  \ENcurve{1,4,0}
\end{endiagram}
\quad
\begin{endiagram}[
   x-label-pos=.7,
   y-label-pos=.7,
   y-label-angle=-90,
   y-label-offset=5pt]
  \ENcurve{1,4,0}
\end{endiagram}
```




Crazy setup:

```
\begin{endiagram}[x-axis={draw=blue,
  dashed,font=\color{green}}]
  \ENcurve{1,4,0}
\end{endiagram}
```




## 4.3 Debugging Information

For precise adjustments of details – particularly with the options and commands described in the next sections – some information is useful that is hidden normally. These options enable access:

`debug` = `true`|`false` Default: `false`

Enable debug mode of ENDIAGRAM.

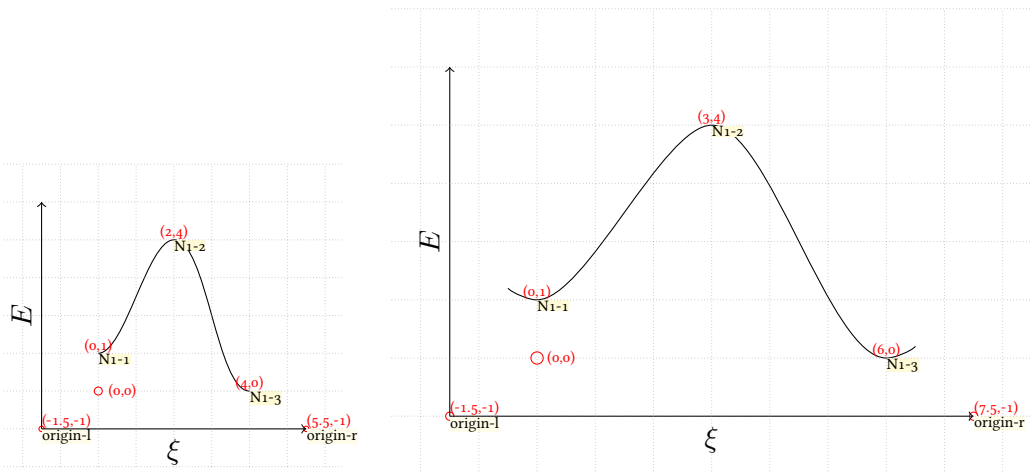
`draft` = `true`|`false` Default: `false`

An alias to `debug`.

`final` = `true`|`false` Default: `true`

The opposite of `draft`.

```
\begin{endiagram}[debug]
  \ENcurve{1,4,0}
\end{endiagram}
\quad
\begin{endiagram}[debug,unit=2em]
  \ENcurve[step=3,minima]{1,4,0}
\end{endiagram}
```




Shown are a grid, the origin and the coordinates and names of the levels. Depending on the commands you're using you get more information. It is described with the commands they belong to.

# 5 The Levels

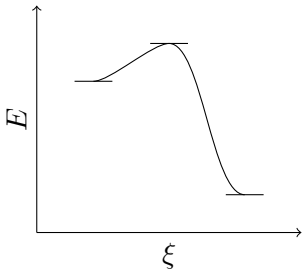
## 5.1 The `\ShowNiveaus` Command

The command `\ShowNiveaus` draws horizontal lines to the levels:

`\ShowNiveaus[`⟨*options*⟩`]`

Draw a visual hint of the different niveaus.

```
\begin{endiagram}
  \ENcurve{3,4,0}
  \ShowNiveaus
\end{endiagram}
```




## 5.2 Customization

A number of options allow fine-tuning:

`length` = {⟨*num*⟩} Default: `1`

`ShowNiveaus` » The length of the lines. ⟨*num*⟩ is a multiple of the SU (see page 4).

`shift` = {⟨*num*⟩} Default: `0`

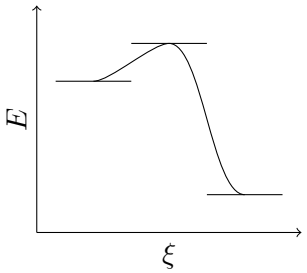
`ShowNiveaus` » Shift to the right (positive values) or the left (negative values). ⟨*num*⟩ is a multiple of the SU.

`tikz` = {⟨*tikz*⟩} (initially empty)

`ShowNiveaus` » Ti*k*Zoptions to modify the style of the lines.

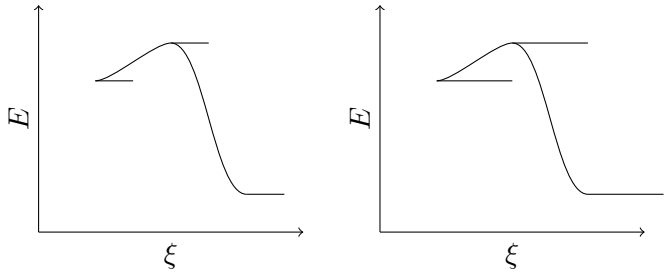
Longer lines:

```
\begin{endiagram}
  \ENcurve{3,4,0}
  \ShowNiveaus[length=2]
\end{endiagram}
```




Without option `shift` the lines are centered to the extrema , *i. e.*, they protrude by half of the value specified with option `length`.

```
\begin{endiagram}
  \ENcurve{3,4,0}
  \ShowNiveaus[shift=.5]
\end{endiagram}
\quad
\begin{endiagram}
  \ENcurve{3,4,0}
  \ShowNiveaus[length=2,shift=1]
\end{endiagram}
```




Maybe the examples in the next section will make it more clear why option `shift` can be useful.

## 5.3 Choose Levels Explicitly

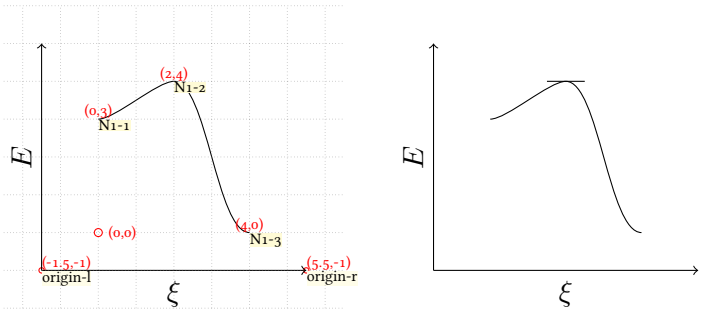
If you don't want to draw a line to every level you can use this option:

`niveau` = {⟨*id1*⟩,⟨*id2*⟩}

`ShowNiveaus` » The ⟨*id*⟩ is the name of the level as shown by the `debug` option, see page 11.

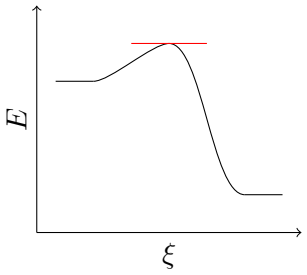
The debug information helps in choosing the right level. The names of the levels follow the scheme `N-`⟨*number of curve*⟩`-`⟨*number of level*⟩.

```
\begin{endiagram}[debug]
  \ENcurve{3,4,0}
\end{endiagram}
\quad
\begin{endiagram}
  \ENcurve{3,4,0}
  \ShowNiveaus[niveau=N1-2]
\end{endiagram}
```




Every level can have a different color, length and shift:

```
\begin{endiagram}
  \ENcurve{3,4,0}
  \ShowNiveaus[length=2,tikz=red,
  niveau=N1-2]
  \ShowNiveaus[niveau=N1-1,shift=-.5]
  \ShowNiveaus[niveau=N1-3,shift=.5]
\end{endiagram}
```



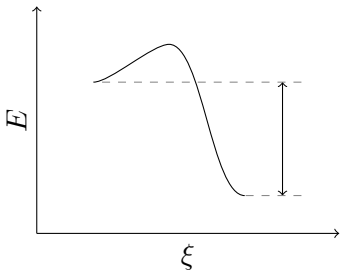

# 6 The Energy Gain

## 6.1 The \ShowGain Command

The command \ShowGain enables you the show the energy gain or loss of the reaction. It is always the difference between the first and the last level.

\ShowGain[⟨*options*⟩]
Draw a visual hint of the energy gain.

```
\begin{endiagram}
  \ENcurve{3,4,0}
  \ShowGain
\end{endiagram}
```




## 6.2 Customization

The command has options to modify the appearance.

ShowGain » tikz = {⟨*tikz*⟩} Default: <->
TikZ options for the vertical line.

ShowGain » connect = {⟨*tikz*⟩} Default: dashed,help lines
TikZ options for the connecting line.

ShowGain » connect-from-line = true|false Default: false
The connecting line starts either at the maximum/minimum or at the line drawn by \ShowNiveaus. This option works with the default values but otherwise can lead to unwanted results. To avoid that you can either set \ShowGain *before* \ShowNiveaus or you need to choose another way.

ShowGain » offset = {⟨*num*⟩} Default: 0
Shifts the vertical line to the right (positive value) or the left (negative value). ⟨*num*⟩ is a multiple of su (see page 4).

ShowGain » label = true|false|⟨*text*⟩ Default: false

Use the default label (true) or an own label (⟨*text*⟩).

ShowGain » label-side = right|left Default: right

The side of the vertical line on which the label should be placed.

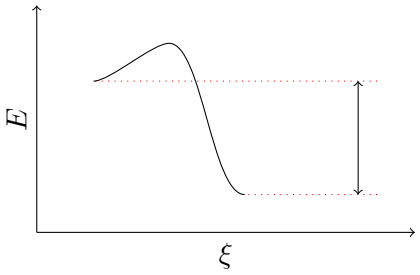
ShowGain » label-pos = {⟨*<value>*⟩} Default: .5

Position at the line. 0 means at the height of $H_1$, *i. e.*, the starting level, 1 means at the height of $H_2$, *i. e.*, the ending level.

ShowGain » label-tikz = {⟨*<tikz>*⟩} (initially empty)

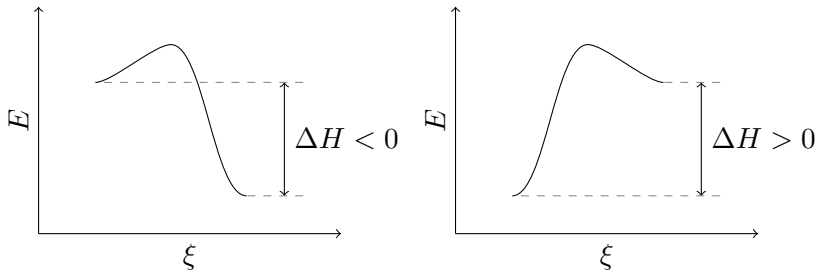
Ti*k*Z options for the label.

```
\begin{endiagram}
  \ENcurve{3,4,0}
  \ShowGain[connect={dotted,red},
  offset=2]
\end{endiagram}
```

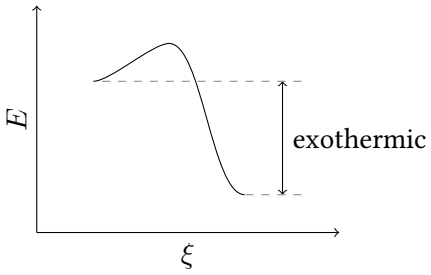



Using the label option:

```
\begin{endiagram}
  \ENcurve{3,4,0}
   \ShowGain[label]
\end{endiagram}
\begin{endiagram}
  \ENcurve{0,4,3}
  \ShowGain[label]
\end{endiagram}
```

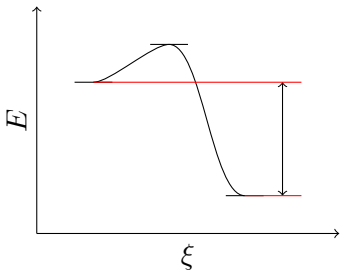


```
\begin{endiagram}
  \ENcurve{3,4,0}
  \ShowGain[label=exothermic]
\end{endiagram}
```



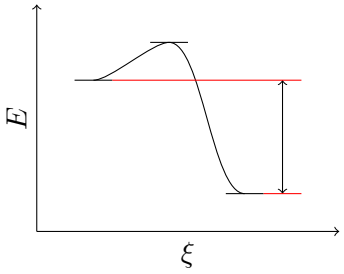

Connecting lines and levels are overlapping:

```
\begin{endiagram}
  \ENcurve{3,4,0}
  \ShowNiveaus
  \ShowGain[connect=red]
\end{endiagram}
```



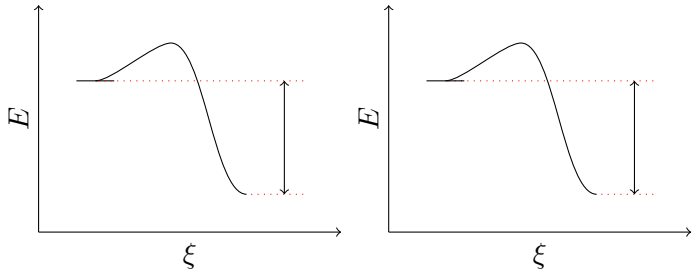

A possible solution:

```
\begin{endiagram}
  \ENcurve{3,4,0}
  \ShowNiveaus
  \ShowGain[connect-from-line,connect=
  red]
\end{endiagram}
```




Better would be to set `\ShowNiveaus` *after* `\ShowGain`, particularly if you're not using the default settings.

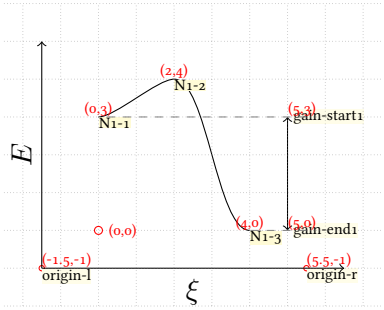
```
\begin{endiagram}
  \ENcurve{3,4,0}
  \ShowNiveaus[niveau=N1-1]
  \ShowGain[connect={red,dotted}]
\end{endiagram}
\begin{endiagram}
  \ENcurve{3,4,0}
  \ShowGain[connect={red,dotted}]
  \ShowNiveaus[niveau=N1-1]
\end{endiagram}
```




## 6.3 Debugging Information

Using the debug option (see page 11) gives you further information:

```
\begin{endiagram}[debug]
  \ENcurve{3,4,0}
  \ShowGain
\end{endiagram}
```




# 7 The Activation Energy

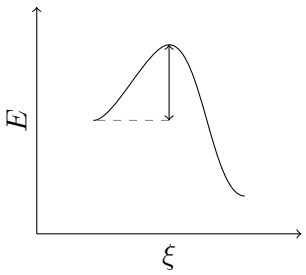
## 7.1 The \ShowEa Command

This command is similar to the commands \ShowNiveaus and \ShowGain.

\ShowEa[⟨*options*⟩]
Draw a visual hint af the activation energy.

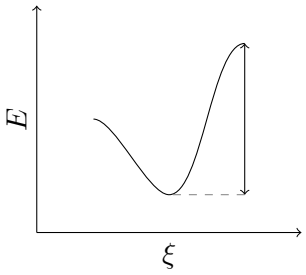
It enables to show the activation energy:

```
\begin{endiagram}
  \ENcurve{2,4,0}
  \ShowEa
\end{endiagram}
```



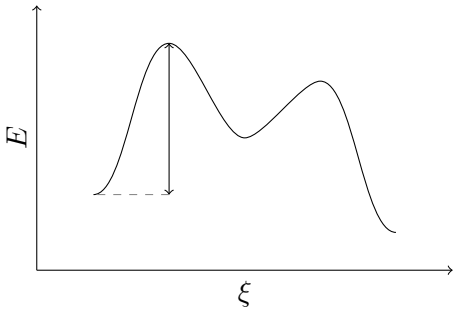

The default behaviour shows the difference between the *first* maximum after a *previous* minimum to that minimum:

```
\begin{endiagram}
  \ENcurve{2,0,4}
  \ShowEa
\end{endiagram}
```




This also holds if there is more than one maximum. How you choose a different one is described in the next section.

```
\begin{endiagram}
  \ENcurve{1,5,2.5,4,0}
  \ShowEa
\end{endiagram}
```




## 7.2 Choose Level Explicitly

The default behaviour is all right if there is only one maximum. If there are more one might want to choose a different one. The following options allow that.

`ShowEa` » `max` = `first|all` Default: `first`

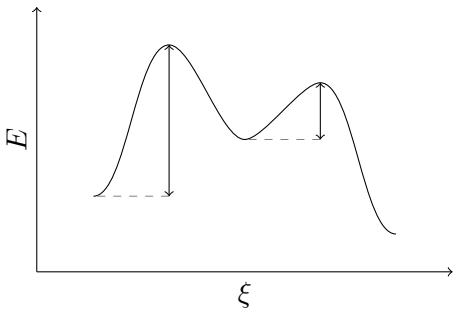
Show the difference to the first maximum or to all maxima.

`ShowEa` » `from` = `{(`⟨*coordinate1*⟩`)to(`⟨*coordinate2*⟩`)}`

Specify the coordinates that should be connected. You can either use the coordinates `(`⟨$x$⟩`,`⟨$y$⟩`)` or the name `(`⟨*name*⟩`)` of the node.

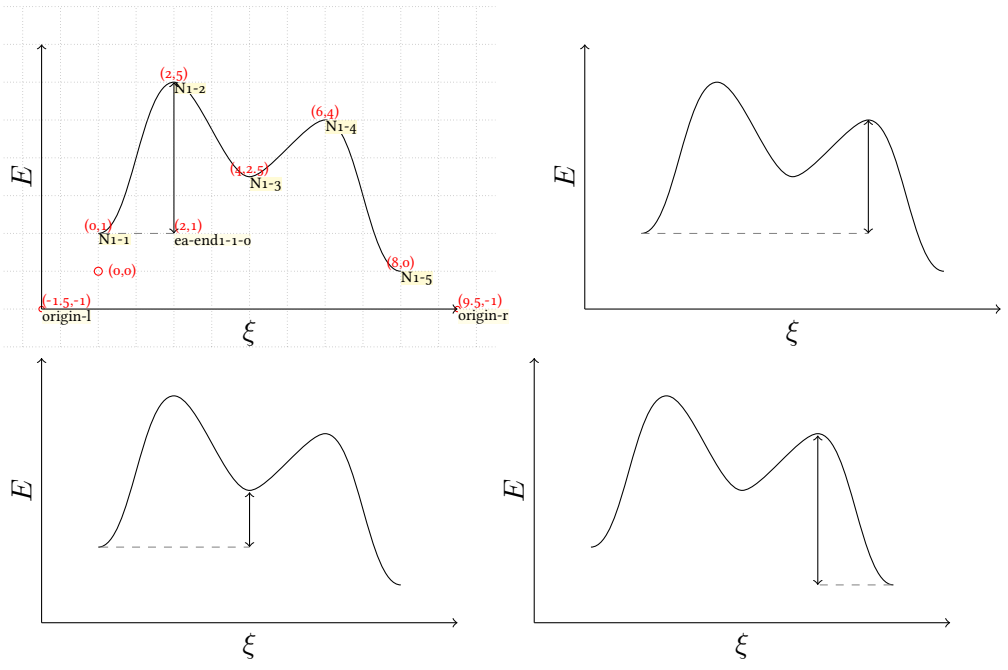
Using `max` = `{all}`:

```
\begin{endiagram}
  \ENcurve{1,5,2.5,4,0}
  \ShowEa[max=all]
\end{endiagram}
```



Since in most cases this won't be what you want you can specify the coordinates yourself. The option debug (see page 11) may help.

```
\begin{endiagram}[debug]
  \ENcurve{1,5,2.5,4,0}
  \ShowEa
\end{endiagram}
\quad
 \begin{endiagram}
  \ENcurve{1,5,2.5,4,0}
  \ShowEa[from={(0,1) to (6,4)}]
\end{endiagram}

\begin{endiagram}
  \ENcurve{1,5,2.5,4,0}
  \ShowEa[from={(N1-1) to (N1-3)}]
\end{endiagram}
\quad
\begin{endiagram}
  \ENcurve{1,5,2.5,4,0}
  \ShowEa[from={(N1-5) to (N1-4)}]
\end{endiagram}
```




In every case the position of the vertical line is determined by the *first* coordinate.

## 7.3 Customization

Again there are a number of options to customize the appearance.

ShowEa » tikz = {⟨*tikz*⟩} Default: <->
TikZ options for the vertical line.

ShowEa » connect = {⟨*tikz*⟩} Default: dashed,help lines
TikZ options for the horizontal line.

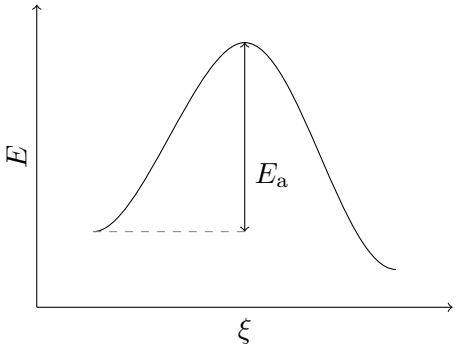
ShowEa » label = true|false|⟨*text*⟩ Default: false
Use the default label ($E_a$) or an own label.

ShowEa » label-side = right|left Default: right
The side of the vertical line where the label should appear.

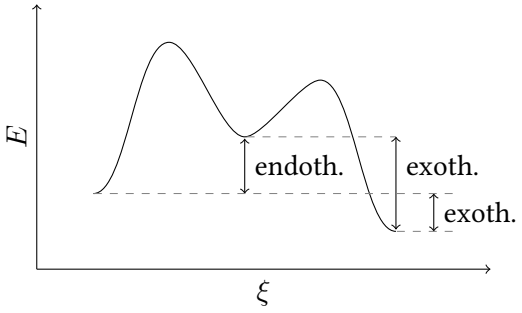
ShowEa » label-pos = {⟨*value*⟩} Default: .5
Determines the vertical position of the label relative to the vertical line. 0 means at the lower end, 1 means at the upper end.

ShowEa » label-tikz = {⟨*tikz*⟩} (initially empty)
TikZoptions for the label.

```
\begin{endiagram}
  \ENcurve[step=4]{1,6,0}
  \ShowEa[label,label-pos=.3]
\end{endiagram}
```



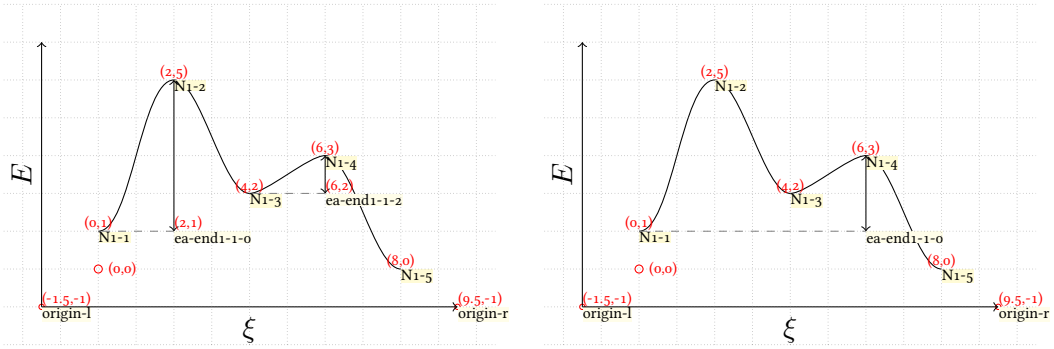

```
\begin{endiagram}
  \ENcurve{1,5,2.5,4,0}
  \ShowEa[
    from    = {(N1-1) to (N1-3)},
    connect = {draw=none},
    label   = endoth.]
  \ShowEa[
    from  = (N1-3) to (N1-5),
    label = exoth.,
    label-pos = .7]
  \ShowGain[label=exoth.]
\end{endiagram}
```



## 7.4 Debugging Information

The `debug` option gives you further information.

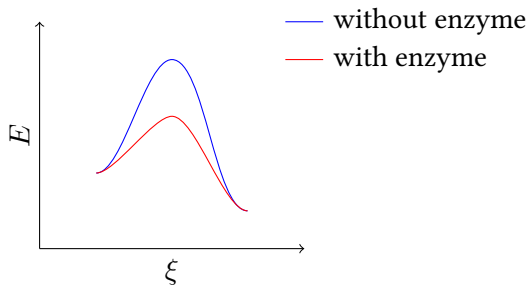
```
\begin{endiagram}[debug]
  \ENcurve{1,5,2,3,0}
  \ShowEa[max=all]
\end{endiagram}
\quad
\begin{endiagram}[debug]
  \ENcurve{1,5,2,3,0}
  \ShowEa[from={(0,1) to (6,3)}]
\end{endiagram}
```




# 8 Several Curves in one Diagram

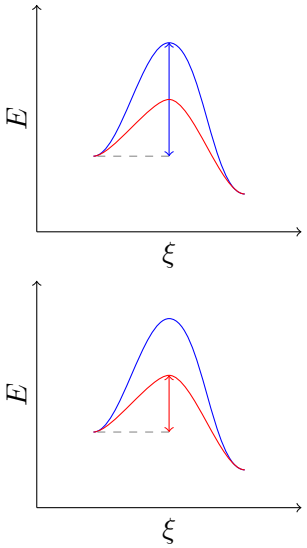
It's easy to draw several curves. You only need to use `\ENcurve` more than once.

```
\begin{endiagram}
  \ENcurve[tikz=blue]{1,4,0}
  \ENcurve[tikz=red]{1,2.5,0}
  \draw[blue] (5,5) -- ++(1,0) node[black,right] {without enzyme};
  \draw[red] (5,4) -- ++(1,0) node[black,right] {with enzyme};
\end{endiagram}
```



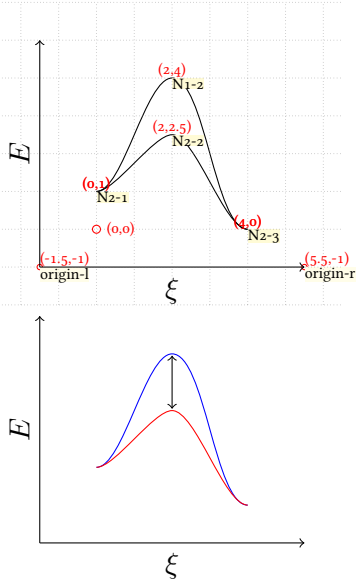

The commands \ShowNiveaus, \ShowGain and \ShowEa always relate to the curve set at last. This means you can use them selectively.

```
\begin{endiagram}
  \ENcurve[tikz=blue]{1,4,0}
  \ShowEa[tikz={blue,<->}]
  \ENcurve[tikz=red]{1,2.5,0}
\end{endiagram}

\begin{endiagram}
  \ENcurve[tikz=blue]{1,4,0}
  \ENcurve[tikz=red]{1,2.5,0}
  \ShowEa[tikz={red,<->}]
\end{endiagram}
```



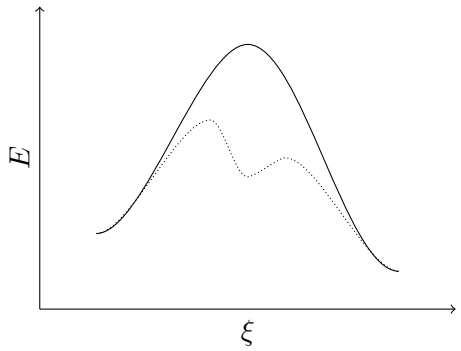

Using more than one curves explains the multiple numbering of the level names:

```
% the names of the levels (N1-1)
% and (N1-3) are hidden behind
% (N2-1) and (N2-3), resp.
\begin{endiagram}[debug]
  \ENcurve{1,4,0}
  \ENcurve{1,2.5,0}
\end{endiagram}

\begin{endiagram}
  \ENcurve[tikz=blue]{1,4,0}
  \ENcurve[tikz=red]{1,2.5,0}
  \draw[<->] (N1-2) -- (N2-2) ;
\end{endiagram}
```




Of course it's possible to choose different options for different curves. This means you can use curves with a different number of maxima.

```
\begin{endiagram}
  \ENcurve[step=4]{1,6,0}
  \ENcurve[
    tikz={densely dotted}]
   {1,4[1],2.5,3[-1],0}
\end{endiagram}
```

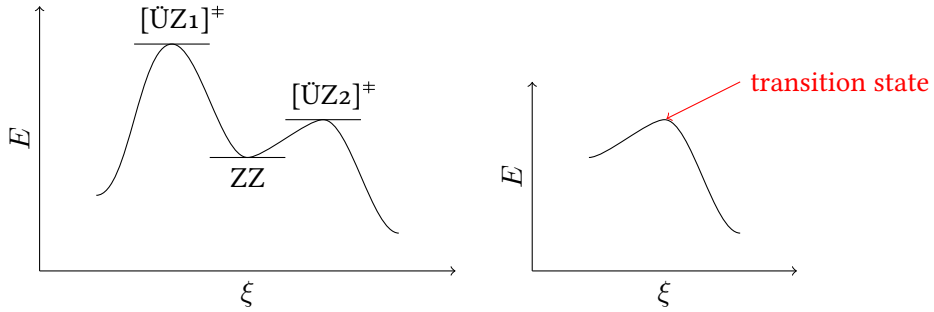



# 9 Usage of TikZ

Since the `endiagram` environment only is a `tikzpicture` environment (well, more or less) you can use TikZ commands inside it. This means you can easily add additional information to the diagram.

```
% needs the package `chemmacros'
\begin{endiagram}
  \ENcurve{1,5,2,3,0}
  \ShowNiveaus[length=2,niveau={N1-2,N1-3,N1-4}]
  \node[above,xshift=4pt] at (N1-2) {[\"UZ1]$^{\transitionstatesymbol}$} ;
```

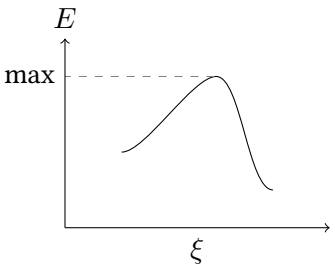
```
  \node[below] at (N1-3) {ZZ} ;
  \node[above,xshift=4pt] at (N1-4) {[\"UZ2]$^{\transitionstatesymbol}$} ;
\end{endiagram}
\quad
\begin{endiagram}
  \ENcurve{2,3,0}
  \draw[<-,red] (N1-2) -- ++(2,1) node[right] {transition state} ;
\end{endiagram}
```




## 9.1 The Origin

The nodes `(origin-l)` and `(origin-r)` are set at the end of the environment. This means they are *not* available inside the `endiagram` environment. If you want to use them you either need to look up their coordinates using the `debug` option (see page 11) …

```
\begin{endiagram}[y-label=above]
  \ENcurve{1,3[.5],0}
  \draw[dashed,help lines]
    (N1-2) -- (N1-2 -| -1.5,-1)
    node[left,black] {max} ;
\end{endiagram}
```



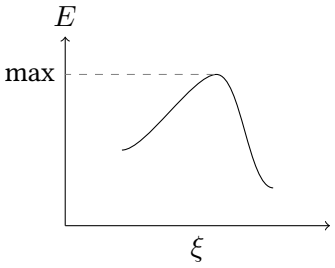

… or use this option:

`tikz` = {⟨*tikz*⟩} (initially empty)

Ti*k*Z options for the `endiagram` environment.

With it you can pass arbitrary Ti*k*Z options to the internal `tikzpicture` environment.

```
\begin{endiagram}[
    y-label = above,
    tikz    = {remember picture}]
  \ENcurve{1,3[.5],0}
\end{endiagram}
\tikz[remember picture,overlay]{
  \draw[dashed,help lines]
    (N1-2) -- (N1-2 -| origin-l)
    node[left,black] {max} ;
}
```

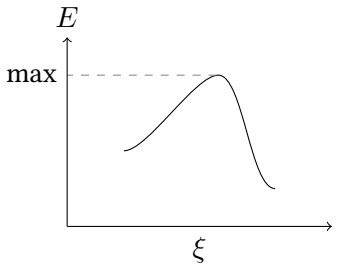



There is an easier way, though: you can use the following command *after* drawing all curves:

`\MakeOrigin`

Helper command to make the origin of the coordinate system known.

```
\begin{endiagram}[y-label = above]
  \ENcurve{1,3[.5],0}
  \MakeOrigin
  \draw[dashed,help lines]
    (N1-2) -- (N1-2 -| origin-l)
    node[left,black] {max} ;
\end{endiagram}
```




# 10 Axes Ticks and Labels

## 10.1 Automatic Ticks

The $y$ axes can get ticks automatically.

`ticks` = `y`|`y-l`|`y-r`|`none` Default: `none`

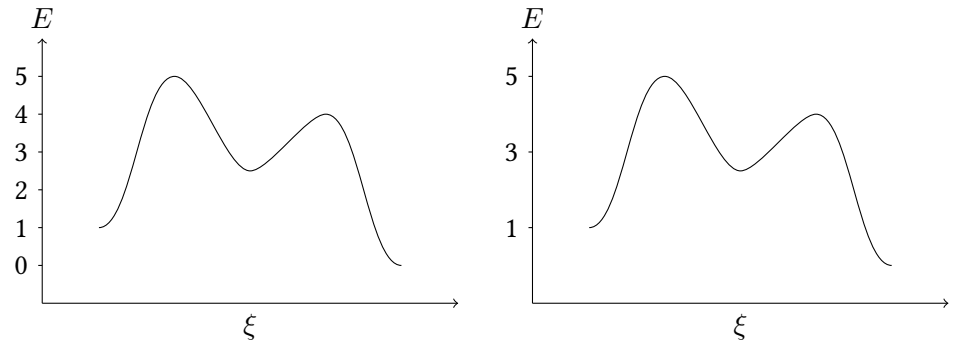
Adds ticks to the specified axes.

`ticks-step` = {⟨*num*⟩} Default: `1`

⟨*num*⟩ is a multiple of the SU. `ticks-step` = `{2}` means that only every second tick is added.

```
\ENsetup{ticks,y-label=above}
\begin{endiagram}
  \ENcurve{1,5,2.5,4,0}
\end{endiagram}
\quad
\begin{endiagram}[ticks-step=2]
```

```
  \ENcurve{1,5,2.5,4,0}
\end{endiagram}
```




These ticks obey the `energy-unit` option, see section 11.

## 10.2 The `\AddAxisLabel` Command

To be able to add labels to the ticks there is the command

`\AddAxisLabel[`⟨*options*⟩`]{(`⟨*point1*⟩`)[`⟨*opt. label*⟩`];(`⟨*point2*⟩`);...}`
Add axis labels to points.

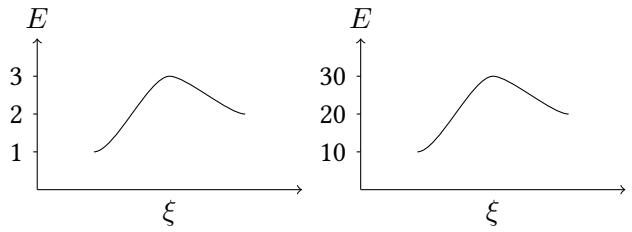
`\AddAxisLabel*[`⟨*options*⟩`]{`⟨*level1*⟩`[`⟨*opt. label*⟩`];`⟨*level2*⟩`;...}`
Add axis labels to levels.

As you can see there are two variants. The first one awaits a list of coordinates in the Ti*k*Z sense. The second awaits $y$ values. Every of these values has an optional argument with which you can specify the label.

The first variant also draws lines between the points specifiad and the $y$ axis. Internally this command calls `\MakeOrigin`, see page 26, which means it should be used *after* drawing all curves.

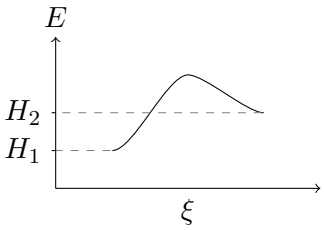
Example for the second variant:

```
\begin{endiagram}[y-label=above]
  \ENcurve{1,3,2}
  \AddAxisLabel*{1;2;3}
\end{endiagram}
\begin{endiagram}[y-label=above]
  \ENcurve{1,3,2}
  \AddAxisLabel*{1[10];2[20];3[30]}
\end{endiagram}
```




Example for the first variant:

```
\begin{endiagram}[y-label=above]
  \ENcurve{1,3,2}
  \AddAxisLabel{(N1-1)[$H_1$];(N1-3)[$H_2$]}
\end{endiagram}
```



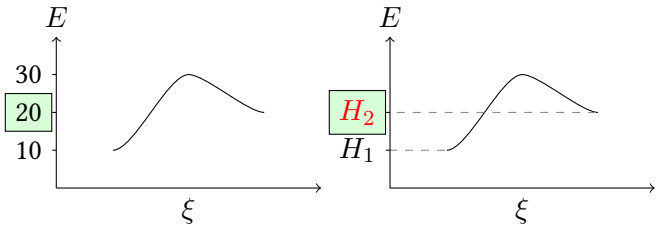

The optional arguments can also get Ti*k*Z options. The description should read:

`\AddAxisLabel[`⟨*options*⟩`]{(`⟨*point1*⟩`)[`⟨*opt. label*⟩`,`⟨*tikz*⟩`];(`⟨*point2*⟩`);...}`
Add axis labels to points.

`\AddAxisLabel*[`⟨*options*⟩`]{`⟨*level1*⟩`[`⟨*opt. label*⟩`,`⟨*tikz*⟩`];`⟨*level2*⟩`;...}`
Add axis labels to levels.

```
\begin{endiagram}[y-label=above]
  \ENcurve{1,3,2}
  \AddAxisLabel*{1[10];2[20,{draw,fill=green!15}];3[30]}
\end{endiagram}
\begin{endiagram}[y-label=above]
  \ENcurve{1,3,2}
  \AddAxisLabel{(N1-1)[$H_1$];(N1-3)[$H_2$,{draw,font=\color{red},fill=green!15}]}
\end{endiagram}
```

---



### 10.3 Customization

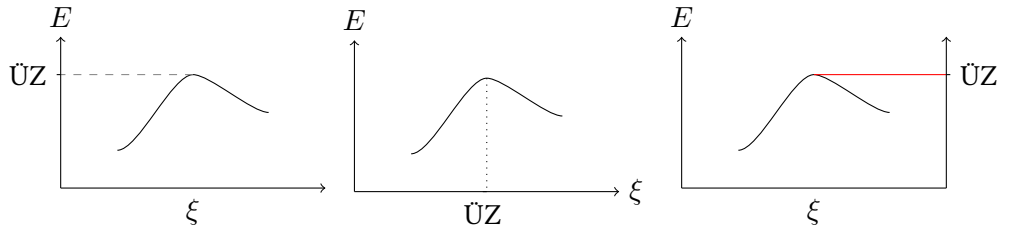
You have several options to customize the labels:

`axis` = `y-l|y-r|x` Default: `y-l`
`AddAxisLabel` » Choose which axis gets the labels.

`connect` = {⟨*tikz*⟩} Default: `dashed,help lines`
`AddAxisLabel` » Change the style of the lines.

`font` = {⟨*commands*⟩} (initially empty)
`AddAxisLabel` » You can add commands like `\footnotesize` and/or `\color{red}` to format the label text.

```
\begin{endiagram}[y-label=above]
  \ENcurve{1,3,2}
  \AddAxisLabel{(2,3)[\"UZ]}
\end{endiagram}
\begin{endiagram}[y-label=above,x-label=right]
  \ENcurve{1,3,2}
  \AddAxisLabel[axis=x,connect=dotted]{(2,3)[\"UZ]}
\end{endiagram}
\begin{endiagram}[axes=all,y-label=above]
  \ENcurve{1,3,2}
  \AddAxisLabel[axis=y-r,connect=red]{(2,3)[\"UZ]}
\end{endiagram}
```




## 11 Actual Values

### 11.1 The Basics

If you want to have a more quantitative diagram or use actual values for the energies you can use these options:

`energy-unit` = {⟨*unit*⟩} (initially empty)
The unit of the energy scale. A unit in the siunitx sense.

`energy-step` = {⟨*num*⟩} Default: `1`
Determines which increment on the energy scale corresponds to the SU.

`energy-zero` = {⟨*num*⟩} Default: `0`

Shifts the origin of the energy scale by ⟨*num*⟩ in multiples of the energy scale.

`energy-unit-separator` = {⟨*anything*⟩} Default: `/`

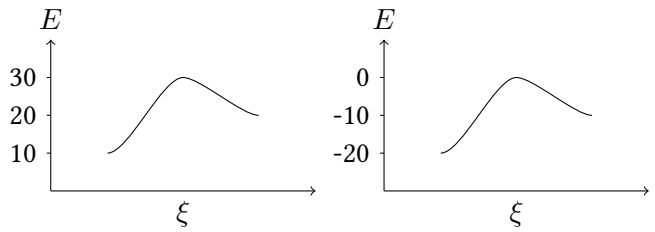
Separates the $y$ axes label from the unit.

`energy-round` = {⟨*num*⟩} Default: `3`

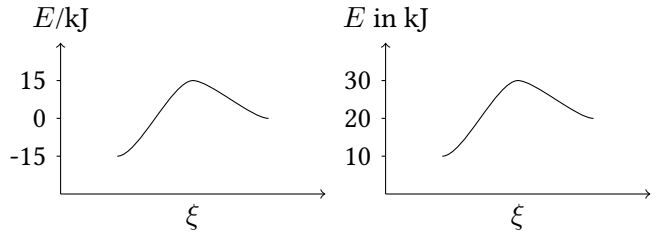
Rounds the value to this number of figures.

Choosing a unit will add ticks and labels to the $y$ axis automatically and has an impact on the commands `\ShowGain` and `\ShowEa`, see section 11.2.

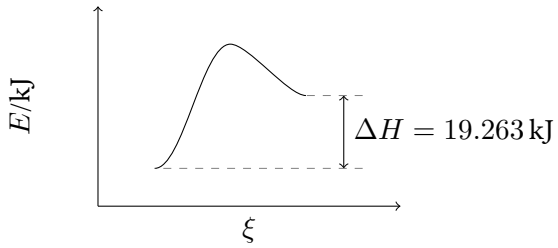
```
\begin{endiagram}[ticks,y-label=above,energy-step=10]
  \ENcurve{1,3,2}
\end{endiagram}
\begin{endiagram}[y-label=above,energy-step=10,energy-zero=30]
  \ENcurve{1,3,2}
  \AddAxisLabel*{1;2;3}
\end{endiagram}
```




```
\begin{endiagram}[
    y-label=above,
    energy-step=15,
    energy-zero=30,
    energy-unit=\kilo\joule]
  \ENcurve{1,3,2}
  \AddAxisLabel*{1;2;3}
\end{endiagram}
\begin{endiagram}[
    y-label=above,
    energy-step=10,
    energy-unit=\kilo\joule,
    energy-unit-separator={ in }]
  \ENcurve{1,3,2}
  \AddAxisLabel*{1;2;3}
\end{endiagram}
```




```
\ENsetup{
  energy-unit=kJ,
  energy-step=10,
  energy-zero=.613,
  y-label-offset=20pt
}
\begin{endiagram}
  \ENcurve{1.0613,4.3465,2.9876}
  \ShowGain[label]
\end{endiagram}
```

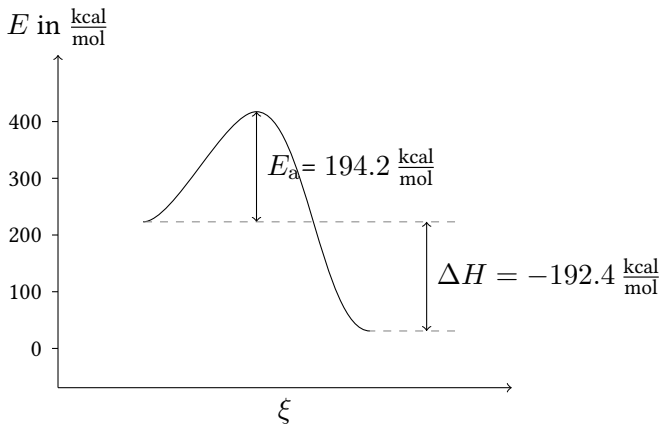



## 11.2 Impact on Other Commands

Using the option `energy-unit` changes the default labels of `\ShowGain` and `\ShowEa`. Now an actual value is shown:

```
% uses \DeclareSIUnit{\calory}{cal}
\sisetup{per-mode = fraction}
\ENsetup{
  energy-step           = 100,
  energy-unit           = \kilo\calory\per\mole,
  energy-unit-separator = { in },
  y-label               = above,
  AddAxisLabel/font     = \libertineLF\footnotesize
}
\begin{endiagram}[scale=1.5]
  \ENcurve{2.232,4.174,.308}
  \AddAxisLabel*{0;1;2;3;4}
```

```
  \ShowEa[label,connect={draw=none}]
  \ShowGain[label]
\end{endiagram}
```

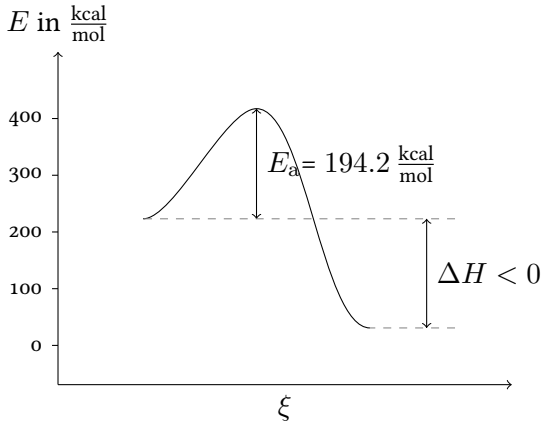



This behaviour can be switched off, though:

`calculate` = `true`|`false` Default: `true`

Switch the calculating of activation energy and energy gain on or off.

```
% uses \DeclareSIUnit{\calory}{cal}
\sisetup{per-mode = fraction}
\ENsetup{
  energy-step           = 100,
  energy-unit           = \kilo\calory\per\mole,
  energy-unit-separator = { in },
  y-label               = above,
  AddAxisLabel/font     = \footnotesize,
}
\begin{endiagram}[scale=1.5,calculate=false]
  \ENcurve{2.232,4.174,.308}
  \AddAxisLabel*{0;1;2;3;4}
  \ShowEa[label,connect={draw=none}]
  \ShowGain[label]
\end{endiagram}
```




## 12 Example

The illustration of the Bell-Evans-Polanyi principle (figure 1) serves as an example for a more complex usage. One reaction is coloured as it an exception to the principle. The figure is a reproduction of a similar figure in [**brueckner** ].

```
% uses the packages `chemmacros', `chemfig' and `libertine'
\setatomsep{1.5em}
\DeclareChemIUPAC\iso{\textit{i}}
\chemsetup[chemformula]{format=\libertineLF}
\ENsetup{
  ENcurve/minima,
  AddAxisLabel/font=\libertineLF\footnotesize
}
\begin{endiagram}[
   tikz         = {yscale=1.5}, scale        = 1.7,
   y-label      = above,        y-label-text = $\Delta H$,
   x-label      = right,        x-label-text = RK,
   energy-step  = 10]
  \ENcurve{0,3.5,1}
  \ENcurve[tikz=red]{0,3.7,.4}
  \ENcurve{0,4.3[.2],2.4}
  \ENcurve{0,4.7[.3],2.7}
  \ENcurve{0,4.9[.35],2.9}
  \ENcurve{0,5.2[.4],3.3}
  \AddAxisLabel*{1;2;3;4;6}
  \AddAxisLabel{
    (N1-1)[0]; (N1-2)[35]; (N2-2)[37]; (N3-2)[43]; (N4-2)[47]; (N5-2)[49];
    (N6-2)[52]
  }
  \draw[right] (N1-3) ++ (1,0)
    node {\small \ch{2 "\chemfig{=_[:30]-[::-60]\lewis{0.,}}~" + N2} } ;
```

```
  \draw[right,red] (N2-3) ++ (1,-.3)
    node {\small \ch{2 "\chemfig{[:-60]*6(=-=-(-\lewis{0.,})=-)}~" + N2} } ;
  \draw[right] (N3-3) ++ (1,-.2)
    node {\small \ch{2 "\tert-\lewis{0.,Bu}~" + N2} } ;
  \draw[right] (N4-3) ++ (1,-.1)
    node {\small \ch{2 "\iso-\lewis{0.,Pr}~" + N2} } ;
  \draw[right] (N5-3) ++ (1,0)
    node {\small \ch{2 "\lewis{0.,Et}~" + N2} } ;
  \draw[right] (N6-3) ++ (1,0)
    node {\small \ch{2 "\lewis{0.,Me}~" + N2} } ;
  \draw[above,font=\fontfamily{fxlf}\selectfont\footnotesize]
   (N1-3) node {10} (N2-3) node[red] {4}
   (N3-3) node {24} (N4-3) node {27}
   (N5-3) node {29} (N6-3) node {33} ;
\end{endiagram}

\setatomsep{2em}
\schemestart
  \chemfig{R-[:30]N=N-[:30]R}
  \arrow{->[$\Delta$]}[,2.1]
  \ch{2 "\lewis{0.,R}~" + N2}
\schemestop
```

## References


[Tan10] Till Tantau. TikZ/pgf. version 2.10, Oct. 25, 2010.
URL: http://mirror.ctan.org/graphics/pgf/.

[Tea] The LaTeX3 Project Team. l3packages.

[Tea13] The LaTeX3 Project Team. l3kernel. version SVN 4582, July 28, 2013.
URL: http://mirror.ctan.org/macros/latex/contrib/l3kernel/.

[Wri13] Joseph Wright. siunitx. version 2.5s, July 31, 2013.
URL: http://mirror.ctan.org/macros/latex/contrib/siunitx/.

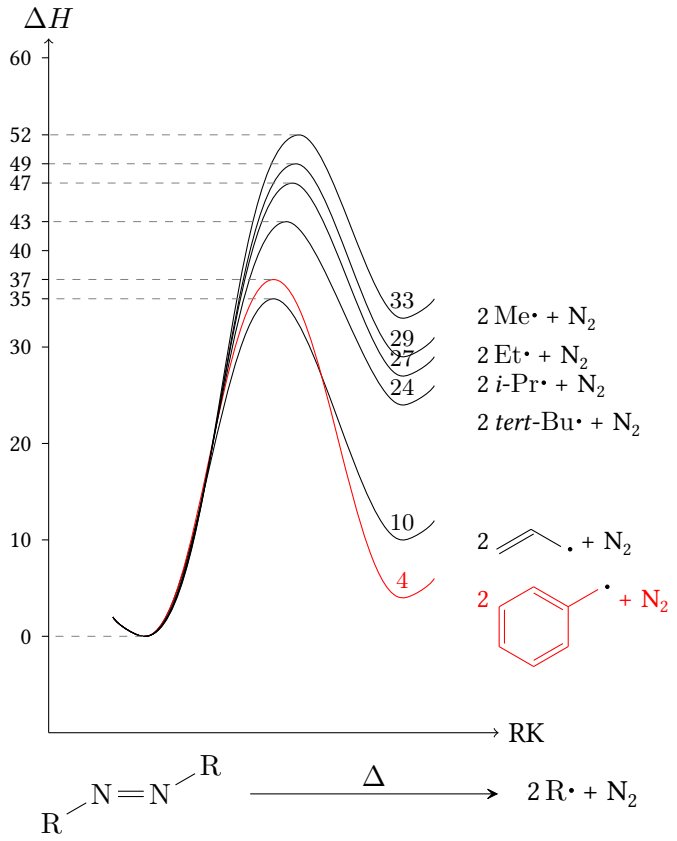



FIGURE 1: Enthalpie-Entwicklung entlang der Reaktionskoordinate bei einer Serie von Thermolysen aliphatischer Azoverbindungen. Alle Thermolysen dieser Serie – mit Ausnahme der farbig hervorgehobenen – folgen dem Bell-Evans-Polanyi-Prinzip [**brueckner** ].

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