EnePro

powerd by python

EnePro Manual

Energy profile generator, version 1.6

---------- Developed and Edited by ----------

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[*EnePro* Website]

https://www.wangzhe95.net/program-enepro

https://github.com/wongzit/EnePro

1. Overview

1.1 About *EnePro*

EnePro is an energy profile generator. *EnePro* is open-source, free, high-efficient, and user-friendly. It supports macOS, Linux and Microsoft Windows operating systems. Source code of *EnePro* is also provided, it can be run with Python IDE.

EnePro is developed with Python 3.9.4, thus, running source code under older version of Python like Python 2 may not work normally. Python external library *openpyxl* is necessary for running *EnePro*, due to Excel processing module is used in the source code.

EnePro can be download at from author's website (https://www.wangzhe95.net/program-enepro) and author's GitHub repo (https://github.com/wongzit/EnePro).

1.2 How it Works

EnePro reads a *Microsoft Excel* (*.xlsx*) input file including the state energy, state labels and state colors. The energy profile would be saved as *ChemDraw* XML file (*.cdxml*), user can open it with *ChemDraw* and make further modification.

1.3 Testing Platform

EnePro has been tested on following platform.

1.3.1 macOS

(1) Mac mini (2020)

CPU: Intel Core i5-8500B 3.00 GHz 6 Cores 6 Threads

Mem: 16 GB 2666 MHz DDR4

GPU: Intel UHD Graphics 630 1536MB

OS: macOS 11.3.1(20E241)

ChemDraw version: 20.0.0.38

(2) MacBook Air (M1, 2020)

CPU: Apple Silicon M1 8 Cores

Mem: 8 GB

GPU: Apple Silicon M1 8 Cores

OS: macOS 11.3.1(20E241)

ChemDraw version: 20.0.0.38

1.3.2 Microsoft Windows

(1) Home-built PC I

CPU: Intel Core i7-9700KF 3.60 GHz 8 Cores 8 Threads

Mem: 16 GB 2666 MHz DDR4

GPU: Nvidia RTX 3060 12GB

OS: Windows 10 Education 20H2

ChemDraw version: 20.0.0.41

(2) Home-built PC II (Physical machine with Windows/Linux dual-boot)

CPU: Intel Core i7-10700 2.90 GHz 8 Cores 16 Threads

Mem: 32 GB 2666 MHz DDR4

GPU: Intel UHD Graphics 630 1536MB

OS: Windows 10 Education 20H2

ChemDraw version: 20.0.0.41

(3) Mac mini (2020) (Running with Parallels Desktop 16)

CPU: Intel Core i5-8500B 3.00 GHz 6 Cores 6 Threads (2 Cores used)

Mem: 16 GB 2666 MHz DDR4 (4 GB used)

GPU: Intel UHD Graphics 630 1536MB

OS: Windows 10 Education 1909

1.3.3 Linux

(1) Home-built PC I (Running with VMware Workstation Player 16)

CPU: Intel Core i7-9700KF 3.60 GHz 8 Cores 8 Threads (6 Cores used)

Mem: 16 GB 2666 MHz DDR4 (12 GB used)

GPU: Nvidia RTX 3060 12GB

OS: CentOS 8.3

(2) Home-built PC II (Physical machine with Windows/Linux dual-boot)

CPU: Intel Core i7-10700 2.90 GHz 8 Cores 16 Threads

Mem: 32 GB 2666 MHz DDR4

GPU: Intel UHD Graphics 630 1536MB

OS: Red Hat Enterprise Linux 8.3

(3) Mac mini (2020) (Running with Parallels Desktop 16)

CPU: Intel Core i5-8500B 3.00 GHz 6 Cores 6 Threads (3 Cores used)

Mem: 16 GB 2666 MHz DDR4 (4 GB used)

GPU: Intel UHD Graphics 630 1536MB

OS: Ubuntu 20.04, Fedora 34 beta

2. Install/Run *EnePro*

2.1 Run with Source Code

If Python IDE is already installed in your computer, you can run *EnePro* with the source code. Python 3.7 or newer is recommended. *EnePro* may not work normally with Python 2. Running of *EnePro* requires the *openpyxl* library, please execute `pip3 install openpyxl` to install it before running *EnePro*. If the `pip3` command is not found, please download the newest Python from https://www.python.org/downloads/ and install.

To run *EnePro* with source code on a Mac/Linux computer, please run following command in terminal:

```
python3 /path_to_EnePro/EnePro_v*_source.py
```

For Microsoft Windows, execute following command in *cmd* or *PowerShell* window:

```
py3 /path_to_EnePro/EnePro_v*_source.py
```

2.2 Run on macOS with Executable File

All executable files are packaged in *execufiles.zip*.

2.2.1 Use Packaged Executable File

The pre-packaged executable file "*EnePro_v*_mac*" should be running normally on macOS 10.15 or newer with Intel and Apple Silicon M1 chip. You can run *EnePro* by double click the icon and *EnePro* will be running in terminal window.

2.2.2 Package Source Code into Executable File

If 2.2.1 is not work for some reason, you can try following steps to package *EnePro* by yourself.

1) Open terminal, execute `pip3 install pyinstaller openpyxl` to install necessary packages. (If the `pip3` command is not found, please download the newest Python from https://www.python.org/downloads/ and install.)
2) Assume the source code file is located "*/home/user/EnePro/EnePro_v*_source.py*", execute command below.

```
pyinstaller /home/user/EnePro/EnePro_v*_source.py --onefile
```

3) An executable file would be generated in *dist* folder. (Only executable file is needed, you can delete other files generated by *pyinstaller*.)
4) Run *EnePro* by double clicking the executable file.

2.3 Run on Linux with Executable File

1) Assume the executable file is located "*/home/user/EnePro/execufiles/EnePro_v*_linux*", run below command to add executable permission to it.

```
chmod +x /home/user/EnePro/execufiles/EnePro_v*_linux
```

2) (Optional) Assume the shell is bash, add below lines to *~/.bashrc* file.

```
alias enepro=/home/user/EnePro/execufiles/EnePro_v*_linux
```

3) After re-entering the terminal, and you can run *EnePro* at any dictionary by execute "`enepro`" command. If you passed the step (2), you need to execute the full path to *EnePro_v*_linux* for running it.

2.4 Running on Microsoft Windows with Executable File

Find "*EnePro_v*_win.exe*" file in program folder, double click it and *EnePro* will be running in command line window. If the Windows Defender stops the *EnePro*, please add the *EnePro* to the safe file list. More details please check: https://faq.nec-lavie.jp/qasearch/1007/app/servlet/relatedqa?QID=018507 and the "Windows User Must Read" file.

3. How to Use

3.1 Prepare Excel Input File

3.1.1 General Structure of Input File

The input file needs to include: (1) color specification, (2) state energy values and (3) state labels.

The **A** column (marked in green) is used for color specification. You need to input the code of color (See section 3.1.2) of which you want to use for the energy surface. From **B** column, energy values need to be inputted in the rows with odd row numbers (marked in blue, 1, 3, 5, ...) and the state labels for each energy state MUST be inputted below the energy values in the rows with even row numbers (marked in red, 2, 4, 6, ...).

Save the input file as Excel *.xlsx* file and submit it to *EnePro* (input the full path to the input file or drag the input file to the command window).

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1		0	35.1288	15.8916	35.547	-43.911	26.7648	-140.097	-54.7842	-141.3516	-50.6022	-137.5878	-180.2442	
2	s	CP1	TS1	CP2	TS2	CP3	TS3	CP4	TS4	CP5	TS5	CP6	CP1	
3								-140.097			-32.6196	-86.9856	-152.643	
4	j							CP4			TS6	CP7	CP1	
5														
6														

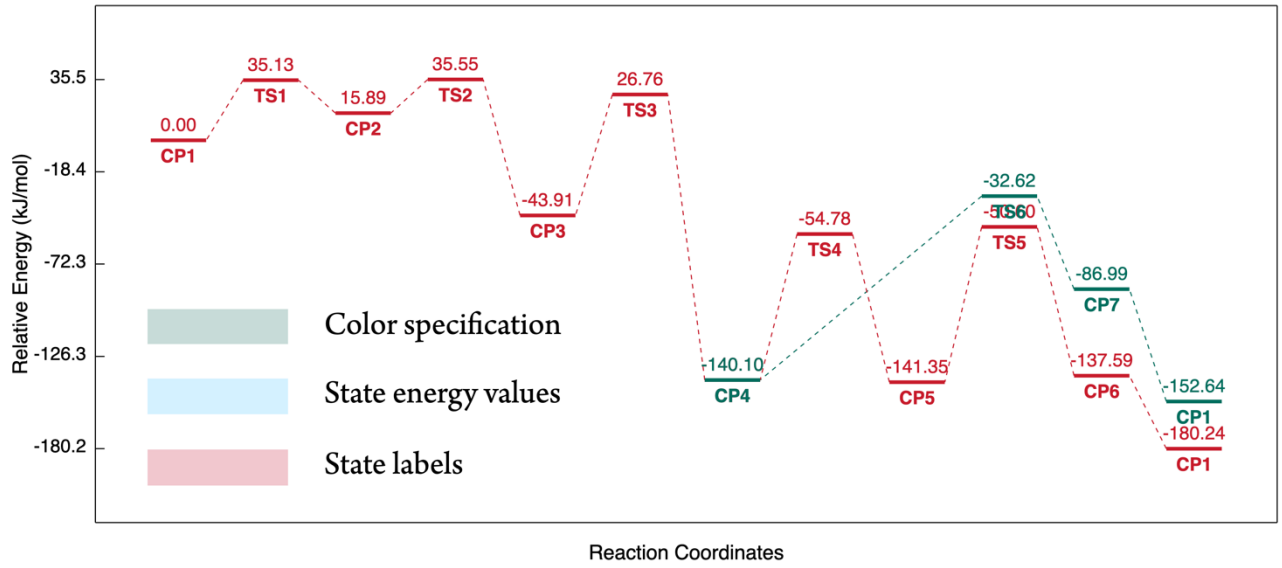

Figure 1. Example input file and its energy profile generated by *EnePro*.

3.1.2 Color Table

EnePro provide 21 colors, including 8 *ChemDraw* default colors and 13 author-selected colors. The full color table is listed in table 1.

Table 1. Color table in *EnePro*.

color	name	code	color	name	code
	Black	*b*		Turquoise	*tu*
	White	*w*		Sky blue	*sb*
	Red	*r*		Dark blue	*db*
	Yellow	*y*		Forest	*fo*
	Green	*g*		Jade	*j*
	Light blue	*lb*		Lime	*l*
	Blue	*bl*		Lemon	*le*
	Purple	*p*		Tangerine	*t*
				Burnt orange	*bo*
				Scarlet	*s*
				Plum	*pl*
				Fuchsia	*f*
				Graphite	*gra*

3.2 Run *EnePro*

*In this section, user inputting is colored in red italic.

1) Run *EnePro*, the *EnePro* will request an Excel input file. You can drag the input file into the command window or input the full path to the input file. Then, press ENTER to submit.

```
Please specify the EnePro input file path:
(e.g.: /EnePro/example/ChemSci2021.xlsx)
/Users/wangzhe/Desktop/ChemSci2021.xlsx
```

2) Following command section would be displayed to set up the plotting parameters:

```
================================================================================
                    Energy profile plotting parameters
--------------------------------------------------------------------------------
```

```
    1 - Decimal digit number for energy value (2)
    2 - Length of energy line (30)
    3 - State span (0.6)
    4 - Energy unit (kJ/mol)
    5 - Use bold font for state label (yes)
=========================================================================
Press ENTER to use current settings, input number to modify the parameters.
```

The parameter in brackets shows current setting, if you want to use current parameters, just press ENTER key. If you want to modify some parameters, please input the menu number, and press ENTER key.

2.1) **Decimal digit number for energy value (2):** specify the number of decimal digits that would be displayed in the energy profile. Default is 2.

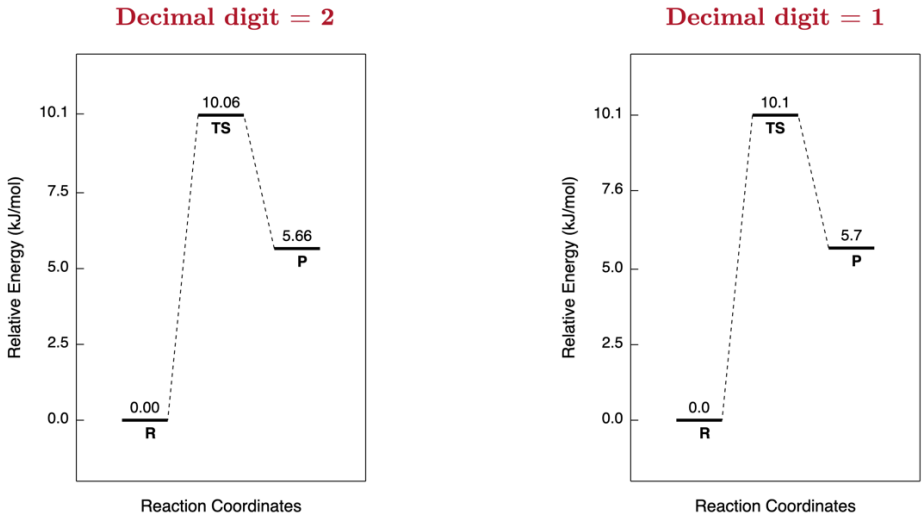

Figure 2. (Left) Two decimal digits and (right) one decimal digit.

2.2) **Length of energy line (30):** Specify the length of bold energy line in energy profile. Default value is 30.

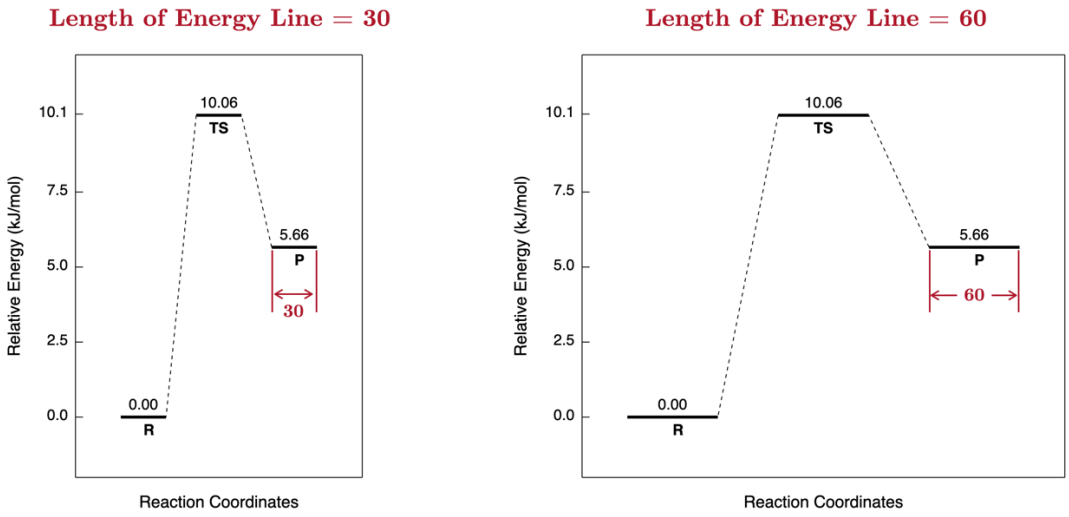

Figure 3. Energy line with length of (left) 30 and (right) 60.

2.3) **State span (0.6):** State span is defined as the ratio of a/b in Figure 4. Large span value will give shorter dash connecting lines. Default value is 0.6.

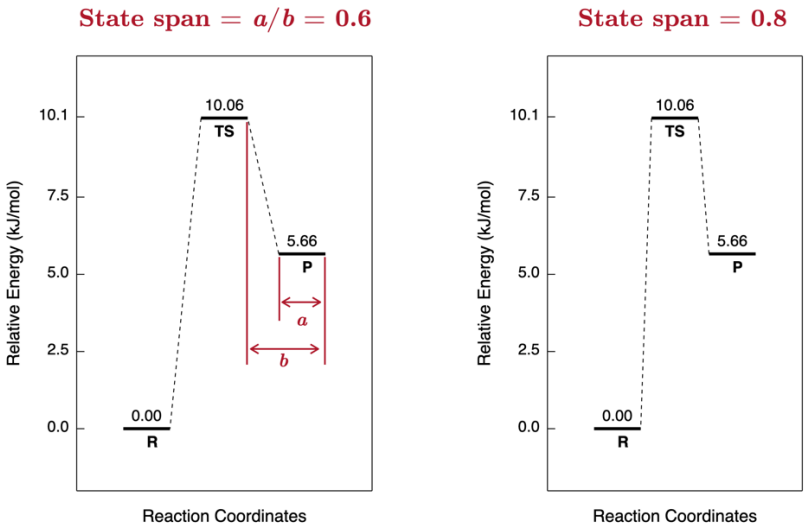

Figure 4. Energy profile with state span of (left) 0.6 and (right) 0.8.

2.4) **Energy unit (kJ/mol):** The default energy unit of *EnePro* is kJ/mol. If you want to use another unit, like kcal/mol, please specify the unit in this menu. Please notice that the energy values will not be changed.

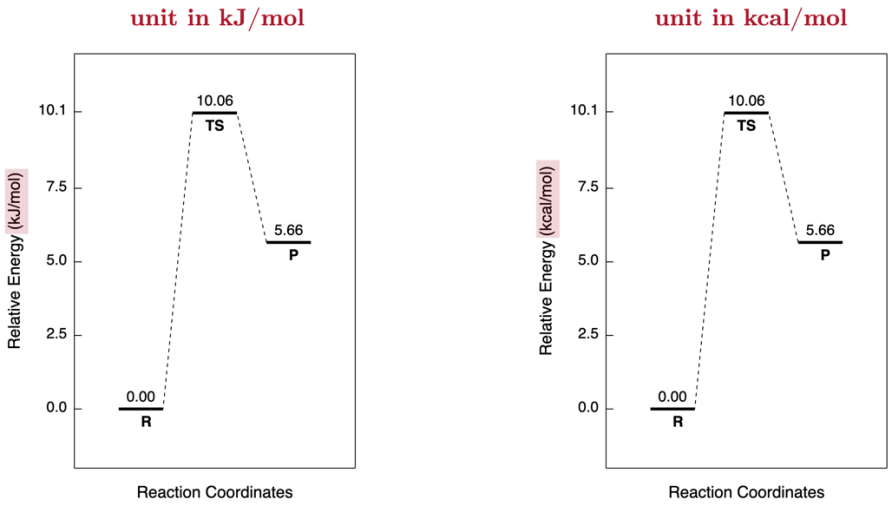

Figure 5. Energy profiles in (left) kJ/mol and (right) kcal/mol.

2.5) **Use bold font for state label (yes):** Specify whether use bold font or not for the state labels. You would enter a second menu screen for modify this parameter.

```
****************************************
1 - Use bold font for energy label
2 - DO NOT use bold font for energy label
Input the menu number:2
```

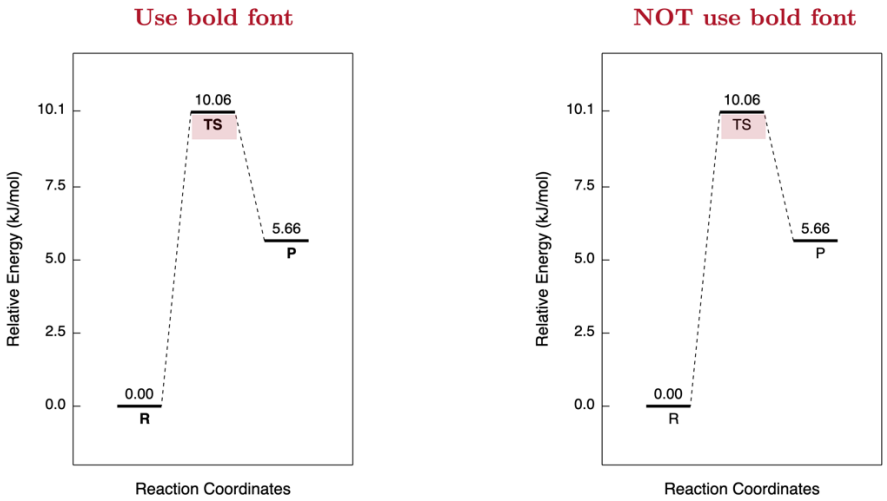

Figure 6. Energy profiles with state labels in (left) bold font and (right) regular font.

3.3 After Running

A *ChemDraw* file named as *EnePro_xxx.cdxml* including energy profile information would be generated in current dictionary. You can open it with *ChemDraw*, check the energy profile and make further modifications. Sometimes the energy values and state labels may overlap with each other, you need to modify the position by hand. I am working on this problem now...

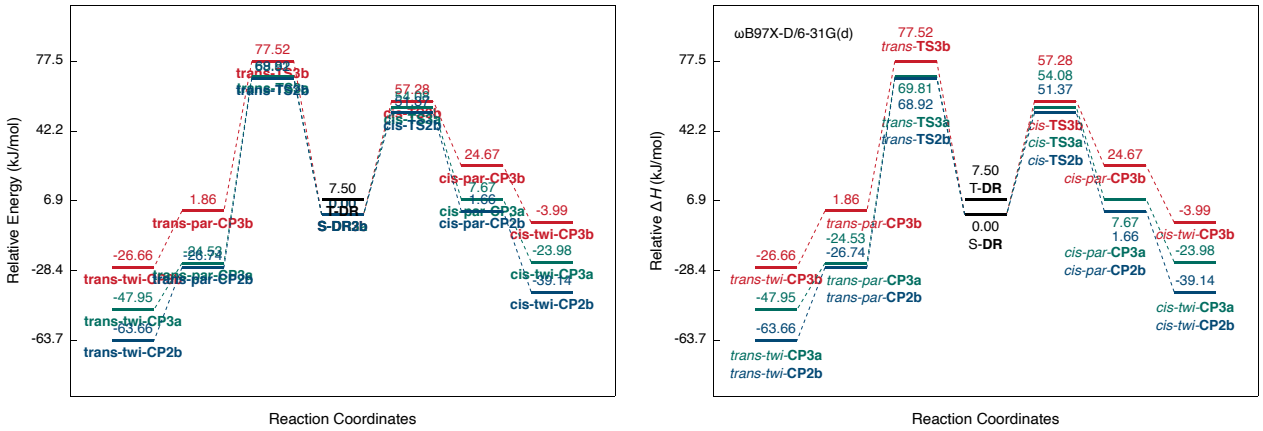

Figure 7. Energy profiles generated by (left) *EnePro* and (right) modified profile.