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# Supplementary Information of rNets: A standalone package to visualize reaction networks.

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## Supplementary notes

#### Note S1: Thermodynamic representation

**Eq S1–3** shows how the activation energy  $(E_{a}^{R})$  and the kinetic constant  $(k^{R})$  are computed for a given reaction R:

$$R: A + B \xrightarrow{[TS]^{\ddagger}} C + D \tag{1}$$

$$E_{\rm a}^{\rm R} = E_{\rm [TS]^{\ddagger}} - (E_{\rm A} + E_{\rm B})$$
 (2)

$$k^{\rm R} = A \exp\left(\frac{-E_{\rm a}^{\rm R}}{k_b T}\right) \tag{3}$$

Where  $E_{\rm A}$  and  $E_{\rm B}$  are the thermodynamic energies of the reactants,  $E_{[\rm TS]^{\ddagger}}$  is the energy of the associated transition state, A is the Arrhenius preexponential factor and  $k_b$  is the Boltzmann constant. In the thermodynamic representation, the width of the edges is computed by normalizing the values of  $\forall {\rm R} \in {\rm N}, \exists k^{\rm R}$ , where N denotes the reaction network.

### Note S2: Kinetic representation

Eq. S4–S7 shows how the net rate  $(r_{net})$  is computed for a given reaction R:

$$\mathbf{R} : a\mathbf{A} + b\mathbf{B} \iff c\mathbf{C} + d\mathbf{D} \tag{4}$$

$$r^{\mathbf{R}} = k^{\mathbf{R}} \cdot [A]^a \cdot [B]^b \tag{5}$$

$$r_{-1}^{\rm R} = k_{-1}^{\rm R} \cdot [C]^c \cdot [D]^d \tag{6}$$

$$r_{\rm net}^{\rm R} = r^{\rm R} - r_{-1}^{\rm R} \tag{7}$$

Here a, b, c, d are the stoichiometric coefficients,  $k_{-1}^{R}$  and  $k^{R}$  are the forward and backward constants, respectively as computed in subsection S1. The symbols [A], [B], [C] and [D] refer to the concentrations of the reactants and the products. The terms  $r^{R}$  and  $r_{-1}^{R}$  are the individual forward and backward rates of the reaction respectively. In determining the kinetic profile of the reaction network, the width of the edges is computed by normalizing the values  $\forall R \in N, \exists r_{net}^{R}$ , where N denotes the reaction network, while their directionality is decided by the sign of  $r_{net}^{R}$ . The directionality of these edges within the network visualization is dictated by the sign of  $r_{net}^{R}$ , indicating the predominant direction of the reaction under the conditions studied.

#### Note S3: Color interpolation

To allow the users to create their custom colorschemes, a color interpolation function has been implemented. **Eq. S8–S12** describe the function implementation.

$$a \in [0, 1] \tag{8}$$

$$Color: (a, a, a) \tag{9}$$

$$Pick: a \to [Color] \to ((Color, Color), a)$$
 (10)

$$InterpolatePair: (Color, Color) \to a \to Color$$
(11)

$$Interpolate : curry \ Interpolate Pair \circ Pick \tag{12}$$

Interpolate works as follow: given a ordered set of colors [Color] and a value a between 0 and 1 (e.g. normalized energy), use Pick to select the color

pair (*Color*, *Color*) and a new value *a* with the projected value between the pair. The output of *Pick* is then used on the *InterpolatePair* function that performs a linear interpolation between the given colors. To obtain more natural color, the interpolation is made in the hue, saturation, lightness (HSL) space, assuring periodicity of the Hue value. Viridis, Magma, Inferno and Cividis colorschemes have been included in our code.

#### Note S4: Luminance selection

To avoid problematic background/label color combinations for the node representation, the relative luminance of the background color is used to chose the label color. Relative luminance (Y) is computed as in **Equation S13**–**S15**, following the directions found in ITU-R BT.709[1]:

$$Y, R, G, B \in [0, 1] \tag{13}$$

$$Color: (R, G, B) \tag{14}$$

$$Y(Color) = 0.2126R + 0.7152G + 0.0722B$$
(15)

Where R, G and B are the red, green and blue component of the given *Color*. Using Y as a threshold, a label color is selected.

#### Note S5: TOML example

```
1 comp_file = "./comp_test.csv"
2 reac_file = "./react_test.csv"
3 out_file = "./test.dot"
4
```

```
5 [graph]
6 kind = "digraph" # Graph kind, digraph almost all the time.
7 colorscheme = ["yellow", "orange", "red", "gold"]
9 [graph.node]
10 font_color = "#000000" # Black
11 font_color_alt = "#fffffff" # White
12 font_lum_threshold = 0.5
13
14 [graph.edge]
15 width = 1 # Minimum width of the arrows
16 max_width = 5 # Maximum width of the arrows
17
18 [graph.opts]
19 rankdir = "TB"
20 \text{ nodesep} = "0.2"
21
22 [graph.node.opts]
23 shape = "plaintext"
24 style = "filled"
25
26 [chem]
_{27} T = 273.15 # Temperature to compute the kinetic constant
```

#### Note S6: Fine-tuning customization

rNets offers extensive customization options for the visualization of reaction networks through the versatile "optional" opts column. This feature enables users to define specific Graphviz attributes for each element within the network—compounds/reactions, represented as nodes and edges respectively. This customization is achieved by specifying key/value pairs, where each pair is linked by an equal sign (e.g., "shape=circle"). For assigning multiple attributes to a single entity, users can separate them with a colon (:) character.

The flexibility afforded by the **opts** column allows for a high degree of personalization in the network's graphical representation. These user-defined attributes have the priority over rNets' default settings. For example, if a user assigns "label=Propylene" to a compound, this custom label will replace the name that would otherwise be sourced from the **name** column. This feature not only enhances the visual appeal but also aids in emphasizing or distinguishing specific elements within the network. Users can employ attributes like "shape=circle" to uniquely identify certain nodes, or use "fillcolor=blue" to bring particular attention to specific reactions.

To ensure users can fully leverage this feature, it is recommended to consult the extensive list of possible Graphviz attributes available in its official documentation.[2] This list provides a comprehensive guide to the various attributes that can be used to modify and enhance the appearance of nodes and edges within the network. By utilizing these attributes, researchers can tailor the network visualization to their specific requirements, making it easier to convey the desired information effectively and intuitively.

## Note S7: The Automated MUltiscale Simulation Environment

The Automated MUltiscale Simulation Environment (AMUSE) is a Python framework able to analyze a reaction network on heterogeneous catalysis from Density Functional Theory (DFT) outputs to macroscopic simulations [3]. First, AMUSE generates automatically the free energy profiles and the reaction mechanism from the CONTCAR and OUTCAR files from the Vienna *Ab-initio* Simulation Package (VASP) [4, 5]. The AutoProfLib and the PreProcessor classes in AMUSE are employed to this end, relying on NetworkX library [6] and functions modified from the Atomic Simulation Environment (ASE) [7] to estimate the free energies of molecules, transition states, and adsorbates.

Then, the mechanistic and energy information contained in the Auto-ProfLib outputs is condensed into kinetic constants, and the time-dependent mass-balance equations for each elementary step in the mechanism are automatically generated and solved using PyMKM, the automated microkinetic framework developed in house and a part of AMUSE [3]. From the mechanism and the energy profiles inputs generated automatically with the AutoProfLib and the initial conditions set by the user (temperature, pressure, initial feed composition...), PyMKM allows the simulation of two different reactors, a differential Plug-Flow Reactor (PFR) and a Continous Stirred Tank Reactor (CSTR). PyMKM relies on the LSODA solver implemented on SciPy [8].

Finally, AMUSE generates automatically the kinetic inputs for Computa-

tional Fluid Dynamics (CFD) simulations [3]. The current version of AMUSE is only able to generate the inputs for the open-source CatalyticFOAM software [9, 10], integrated into OpenFOAM [11], a general framework for CFD simulations. The output of the CFD simulations can be compared one-to-one with experiments in terms of selectivity and conversion in all the domains of the reactor [3].

#### Note S8: Density functional theory

DFT simulations for the cyclooctene epoxy alcohol [12] (knowledge graph example) were carried out with the Gaussian09 [13] software package, with a B97D3 [14, 15] hybrid functional and a standard Pople 6-311G(d,p) [16, 17] basis set for all atoms. The SMD model [18] was used to model implicit solvation, using the predefined parameters for butanone (experimental solvent). Gibbs free energies were computed using the rigid rotor harmonic oscillator (RRHO) model at 298.15 K and 1 atm.

The DFT input for AMUSE was taken from previous computational studies [19, 20]. DFT simulations were performed with the Vienna Ab Initio Simulation Package [4] and the Perdew–Burke–Ernzerhof (PBE) functional [21]. Core electrons were treated with the Projector Augmented Wave (PAW) method [22, 23] and valence electrons were expanded with plane waves. The cut-off energy was set to 450 eV, and the Brillouin zone was sampled using a 3x3x1 k-points mesh [19, 20].

The DFT simulations for the imine condensation were carried out with the same methodology as in our original paper [24]. The values used to generate Figure 3 were directly extracted from our previous publication [24]. Single Point calculations using Gaussian16 [25] using DRACO-corrected [26] atomic radii were carried out at the same theory level, B3LYP-D3/cc-pVTZ with SMD implicit solvation for dichloromethane. [27–31]. An electrostatic scaling factor of 1.2 was used (matching the default values of the software used in the development of DRACO). To compute the adjusted radii the version 1.0.0 of DRACO was used with the default charge model ('ceh') for smd and dichloromethane.

#### Note S9: Energy-based reaction network

Figure SS2 highlights the importance of conveniently defining the visible attribute: the presence of very highly connected nodes for  $CO_2$ , TMA and TMABr clearly hinders the interpretability of the overall network. In contrast, the simplified network showcased in the main text (Figure 4) enables the actual catalytic mechanism to be understood, just by omitting these common species.

#### Note S10: Pykinetic microkinetic simulations

Pykinetic [32] is a python library and two command-line applications ('pykineticmodel' and 'pykinetic-scan') to generate self-contained scripts independent of pykinetic to carry out microkinetic and kinetic simulations, typically used for facilitate the creation and scripting of kinetic models from non-periodic DFT calculations. The command-line applications take two input files similar to the input files of rNets, one containing the energetics of all species and another one containing the reactions and barriers. Its python API also allows the creation of kinetic models through python scripting. Pykinetic currently supports two possible output programming languages for the self-contained model: Python and C++. For the present work, the Python option was used which relies on the LSODA solver as implemented on SciPy [8]. The kinetic simulations using the DRACO-corrected energies share the same model details as our previous work [24], fully detailed in the corresponding SI. The only differences are the DFT energies used and the scan of the systematic bias. The energies used in the present work were corrected using Single Point calculations with adjusted radii as indicated in **Note S8**. The interval of scanned bias values was [3.0,5.0] kcal/mol in steps of 0.1 kcal/mol. These values are shown in kJ/mol in the main text at Figure 7.

## Figures



Figure S1: Examples of the Viridis colorscheme and custom gradients using the interpolation algorithm within the CIE-Lab colorspace. The examples are inspired in the Matplotlib colorschemes representation.



Figure S2: Visualization of the reaction network for  $CO_2$  fixation on an epoxy alcohol cyclooctene derivative, without defining any species to be hidden. The magnitude of the energy barriers for each elementary step is represented by the color and the thickness of the arrows, while the color of the nodes represents the stability of the intermediates.



Figure S3: Complete reaction network of the imine condensation without any correction in DCM between benzaldehyde (A) and n-butylamine (N). The adduct of 'X' and 'Y' is represented as '[X+Y]'. Water, the hemiaminal intermediate and the product Imine are represented as 'W', 'H' and 'I' respectively. The magnitude of the energy barriers for each elementary step is represented by the color and the thickness of the arrows, while the color of the nodes represents the stability of the intermediates. The color scale goes from dark, corresponding to low energies (thus high stability) and barriers to light colors, indicating unstable intermediates and high barriers.



Figure S4: Complete reaction network of the imine condensation with standard state correction and a bias of 13.38 kJ/mol per DFT calculation in DCM between benzaldehyde (A) and n-butylamine (N). The adduct of 'X' and 'Y' is represented as '[X+Y]'. Water, the hemiaminal intermediate and the product Imine are represented as 'W', 'H' and 'I' respectively. The magnitude of the energy barriers for each elementary step is represented by the color and the thickness of the arrows, while the color of the nodes represents the stability of the intermediates. The color scale goes from dark, corresponding to low energies (thus high stability) and barriers to light colors, indicating unstable intermediates and high barriers.



Figure S5: Complete Imine condensation reaction with an energy bias (4.2 kcal/mol) from the DRACO-corrected DFT energy values and reference state correction to 1M at a simulation time of 10min. The thickness of the arrows represents the net rate for each elementary step, and the orientation of the arrow indicates the direction of the reaction, while the color of the nodes represents the concentration of the intermediates. A dark color represents a low or null concentration while a bright color corresponds to a high concentration.



Figure S6: Complete Imine condensation reaction with an energy bias (4.2 kcal/mol) from the DRACO-corrected DFT energy values and reference state correction to 1M at a simulation time of 40min. The thickness of the arrows represents the net rate for each elementary step, and the orientation of the arrow indicates the direction of the reaction, while the color of the nodes represents the concentration of the intermediates. A dark color represents a low or null concentration while a bright color corresponds to a high concentration.

## Tables

Column name	Value	Behavior	Required
name	Text	Text on the node	Yes
energy	Real	Energy of the compound	Yes
fflags	b, i and u	Format of the text label	No
visible	t, f or grey	Visibility of the node	No
conc	Real	Concentration	No
opts	key=value	Graphviz node attributes	No

Table S1: Possible column names and values for the compounds file.

Table S2: Possible column names and values for the reactions file.

Column name	Value	Behavior	Required
cleft	Text	Compound at left	>=1
$\operatorname{cright}$	Text	Compound at right	>=1
energy	Real	Transition state energy	No
visible	t, f or grey	Visibility of the edges	No
opts	key=value	Graphviz edge attributes	No
direction	->, <-, <->	Direction of the reaction	No
name	Text	Name of the reaction	No

Table S3: Node configuration values. Opts. default options are specified in rNets documentation.

Option name	CLI	Value	Behavior	Default
box_tmp	N/A	Text	HTML node box	Simple box
$font\_color$	-f	Text (Color)	Font color	Black
$font\_color\_alt$	-a	Text (Color)	Bright font color	White
$font\_lum\_threshold$	-1	Real $[0,1]$	Luminance thresh.	None
opts	-no	[key=value]	Graphviz opts.	Doc.

Table S4: Edge configuration values. Opts. default options are specified in rNets documentation.

Option name	CLI	Value	Behavior	Default
solid_color	-ec	Text (Color)	Solid edge color	None
width	-W	Real	Edge (min) width	1.
$\max_{width}$	-mw	Real	Edge max width	5.
opts	-eo	[key=value]	Graphviz opts.	Doc.

Table S5: Graph configuration values. Opts. default options are specified in rNets documentation.

Option name	CLI	Value	Behavior	Default
kind	-k	Text	Graph kind	Digraph
colorscheme	-с	$Text \mid [Color]$	Graph colorscheme	Viridis
$color_offset$	-off	(Real, Real)	Color offset	(0.,0.)
opts	-go	[key=value]	Graphviz opts.	Doc.

Table 50. Chemical configuration values	Table S6:	Chemical	configuration	values
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Option name	CLI	Value	Behavior	Default
Т	-T	Real	React. Temperature	273.15
$e\_units$	-u	Text	Energy units	eV
kb	-kb	Real	Boltzmann Const.	8.62 E-5
А	-A	Real	Pre-exp. factor	1E13

Table S7: Intermediate labels for **Figure 4**.

Label	Intermediate	Label	Intermediate
i0	Pd	i9	CHOH*
i1	$2H^*$	i10	$\mathrm{CHOH}^*+2\mathrm{H}^*$
i2	$\mathrm{CO}_2^*+2\mathrm{H}^*$	i11	$\mathrm{CH}_{2}\mathrm{OH}^{*} + \mathrm{H}^{*}$
i3	$\mathrm{COOH}^* + \mathrm{H}^*$	i12	$CH_3OH^*$
i4	$\mathrm{CO}^* + \mathrm{OH}^* + \mathrm{H}^*$	i13	$\mathrm{CHO}^* + \mathrm{H}^*$
i5	$\mathrm{CO}^* + \mathrm{H}_2\mathrm{O}^*$	i14	$CH_2O^*$
i6	$\mathrm{CO}^* + \mathrm{H}_2\mathrm{O}_{(g)}$	i15	$\mathrm{CH}_2\mathrm{O}^*$ + 2H*
i7	$\rm CO^*$ +2H*	i16	$\mathrm{CH}_3\mathrm{O}^* + \mathrm{H}^*$
i8	$\rm COH^* + H^*$		

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