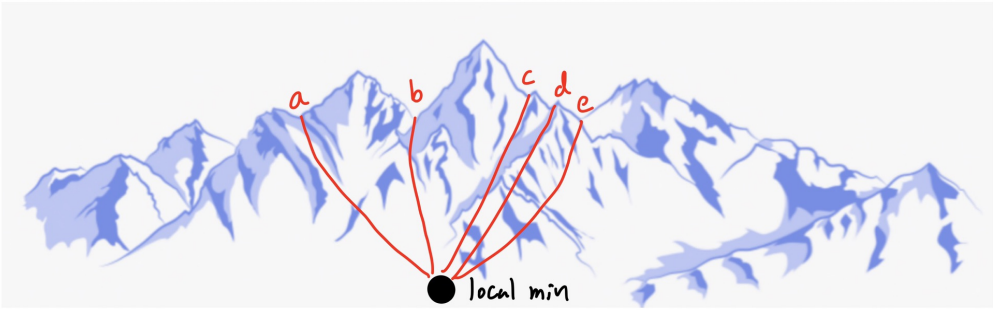
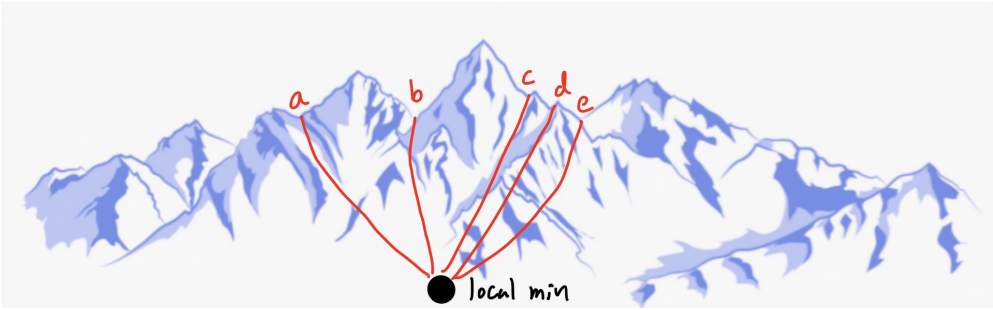
Additive energy functions have predictable landscape topologies



Henry Adams, University of Florida

Joint with Brittany Story, Biswajit Sadhu, Aurora Clark

Additive energy functions have predictable landscape topologies



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Thanks for some of the slides!

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Additive energy functions have predictable landscape topologies

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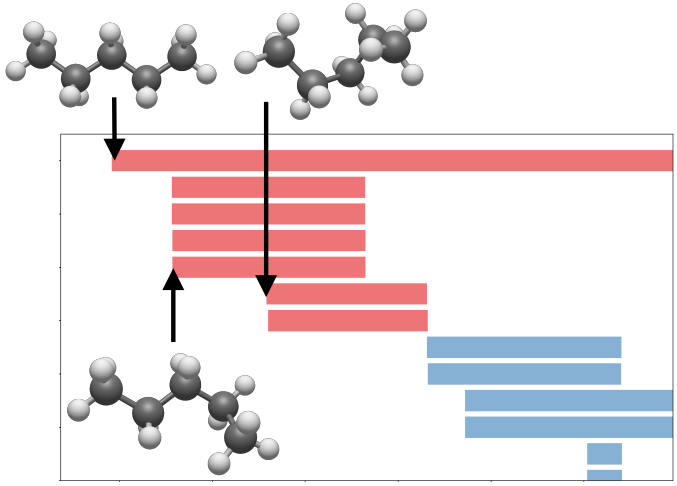
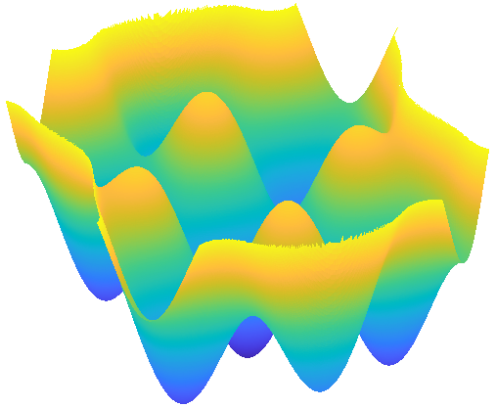
Representations of Energy Landscapes by Sublevelset Persistent Homology: An Example with n-alkanes





Henry Adams, Colorado State University, DELTA NSF #1934725

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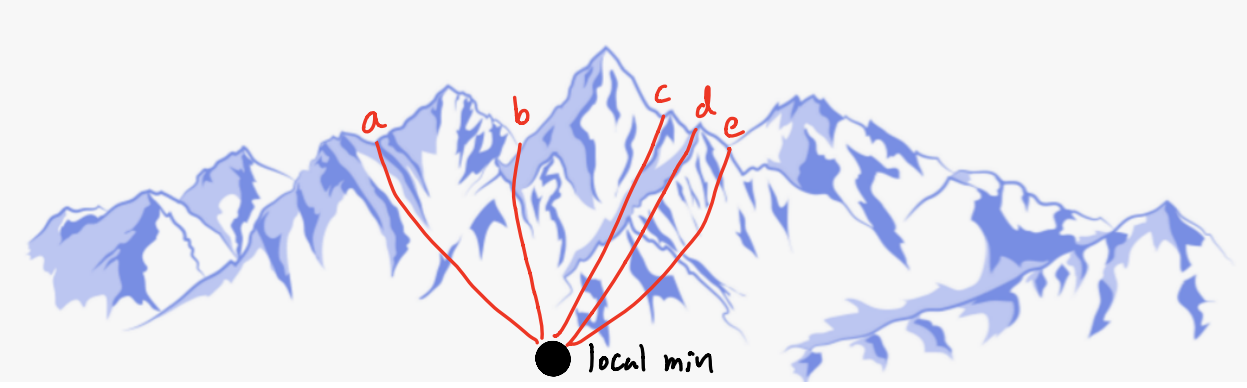
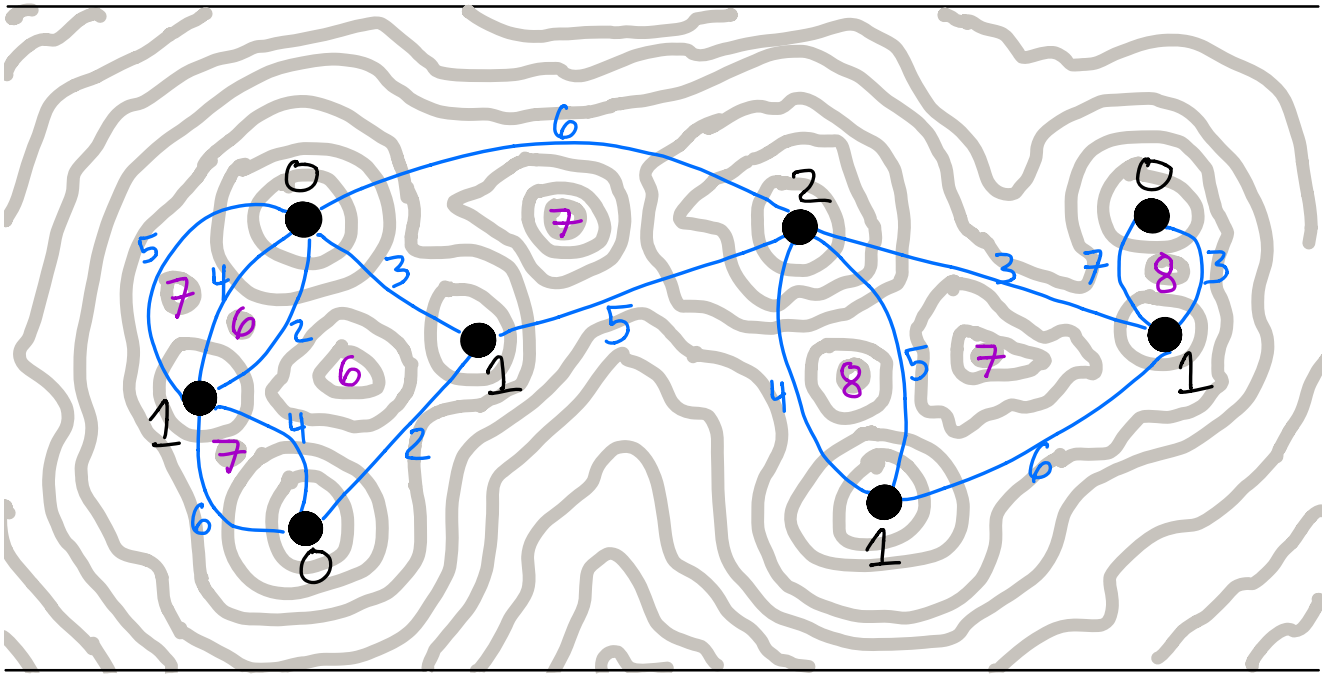
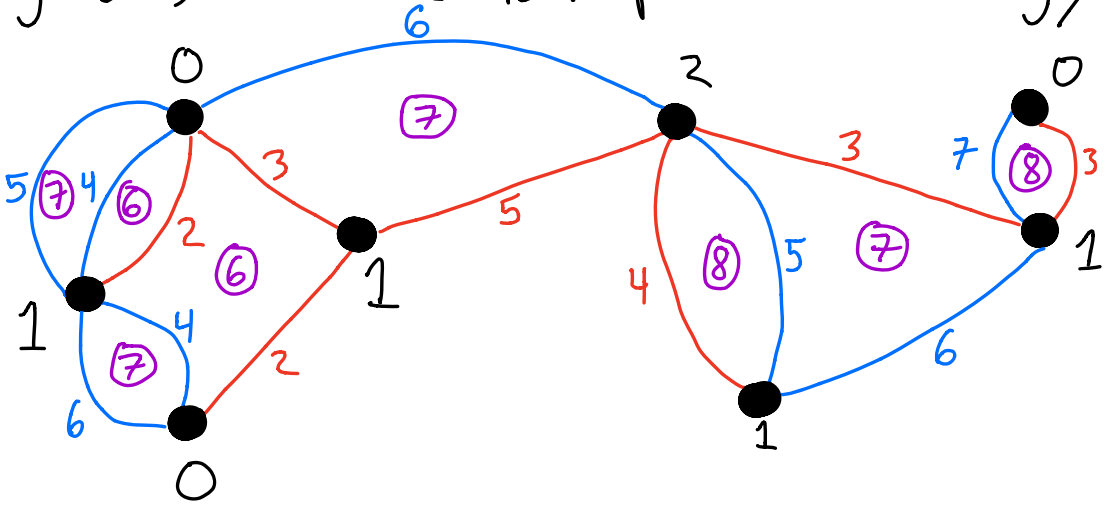

a
b
c
d
e
local min

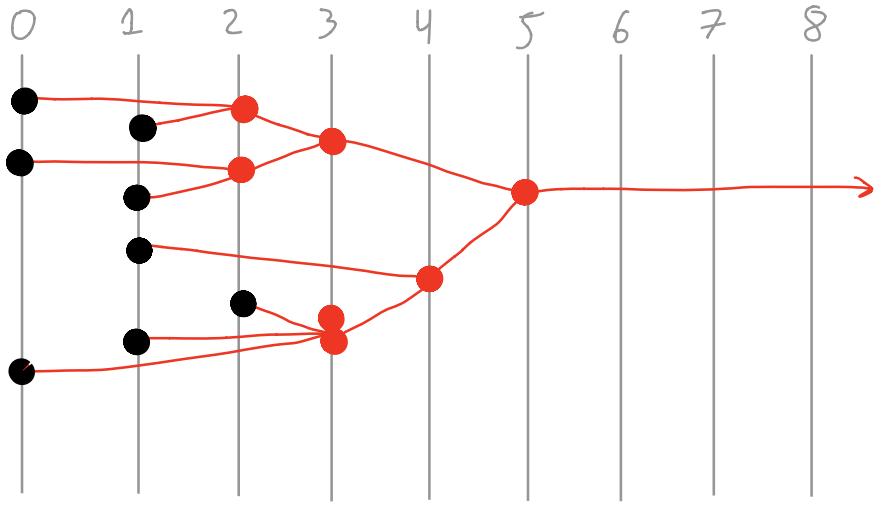
Merge trees and sublevelset persistent homology



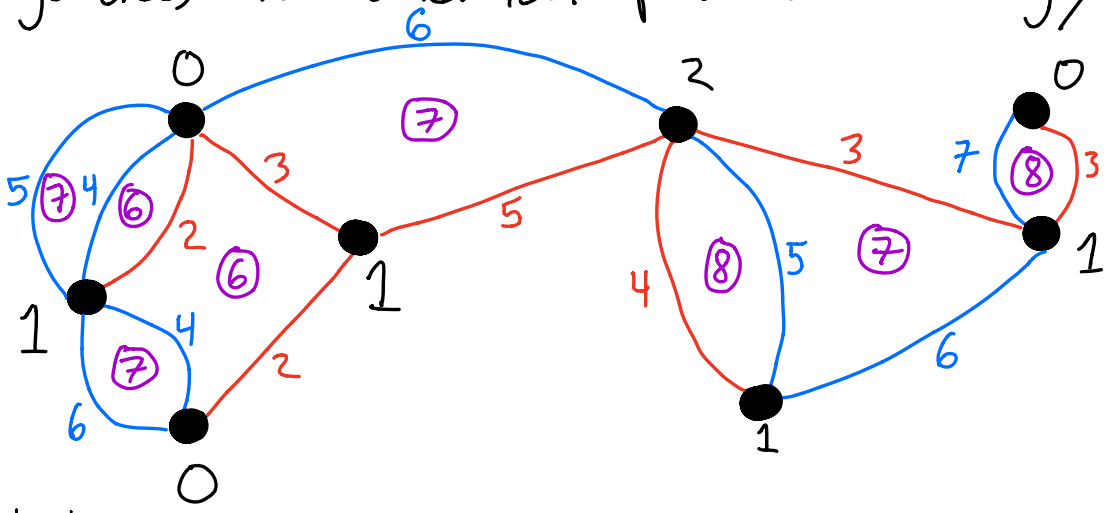
Merge trees and sublevelset persistent homology



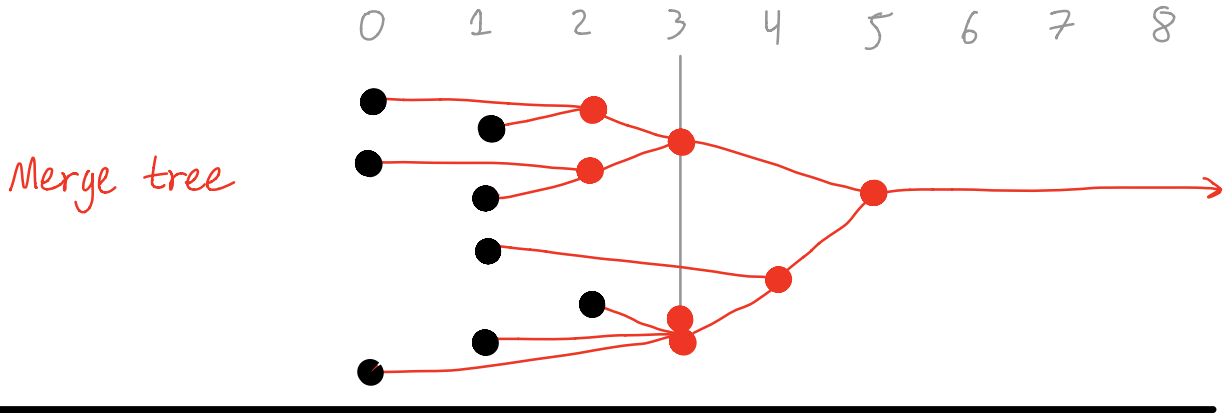
Merge tree

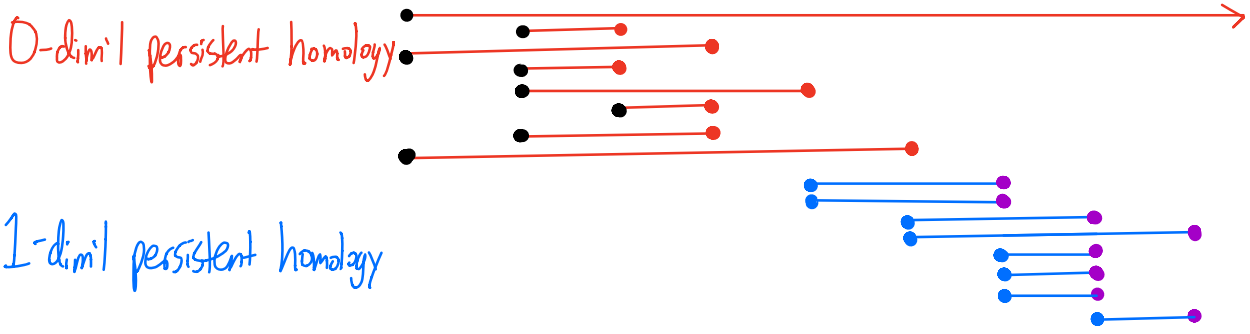


Merge trees and sublevelset persistent homology

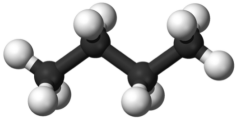


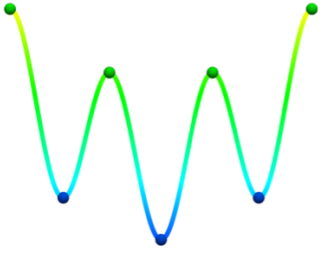
- local minima
- index 1 saddle that merges two components
- index 1 saddle that creates a loop
- index 2 critical point





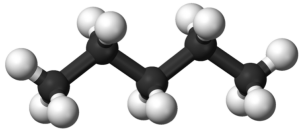
Butane

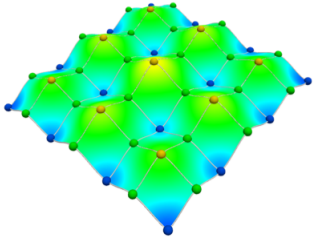




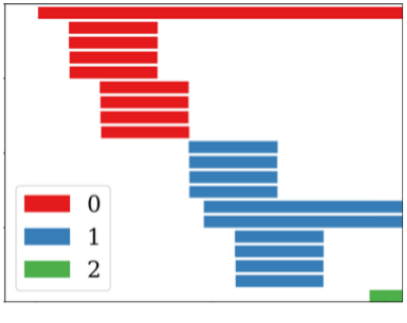
Energy $f: S^1 \to \mathbb{R}$

Pentane

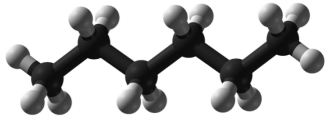


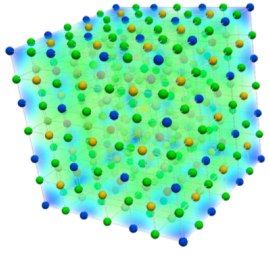


Energy $f(\phi_1) + f(\phi_2)$

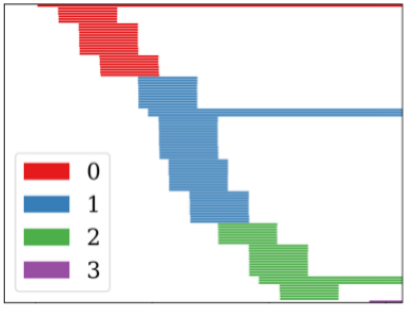


Hexane

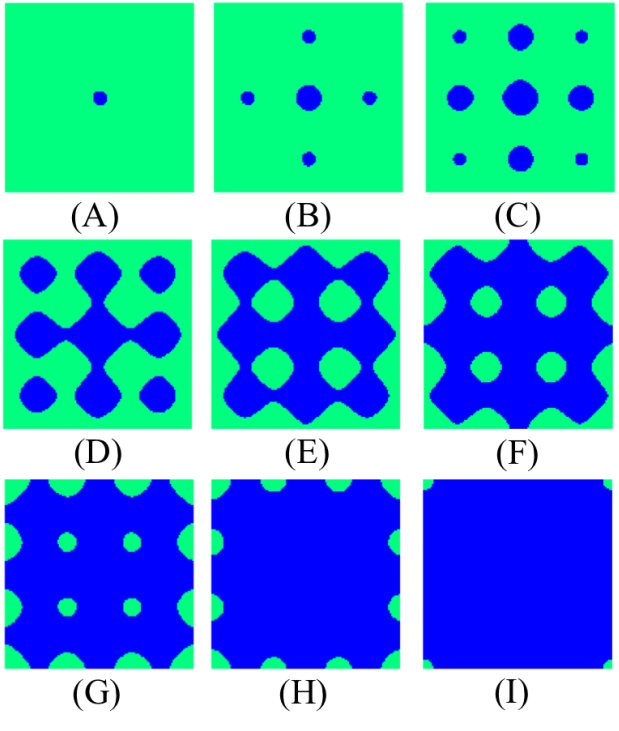


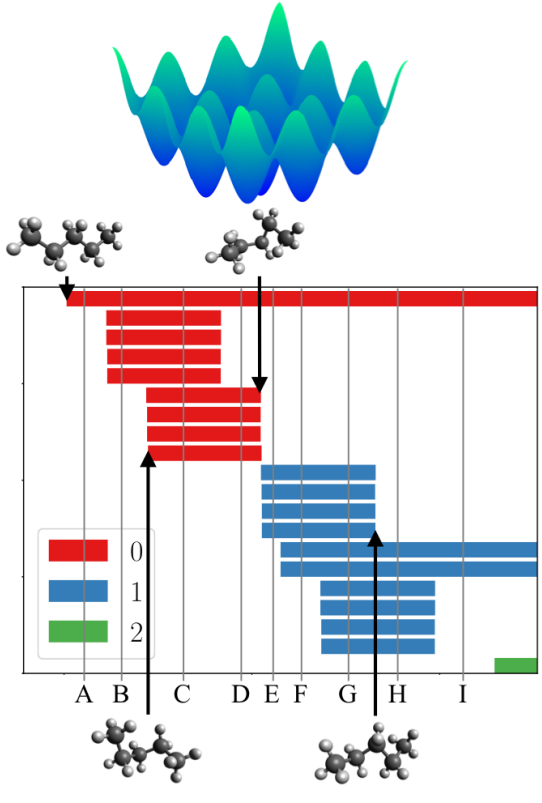


Energy $f(\phi_1) + f(\phi_2) + f(\phi_3)$



Sublevelset persistent homology of pentane (OPLS-UA)





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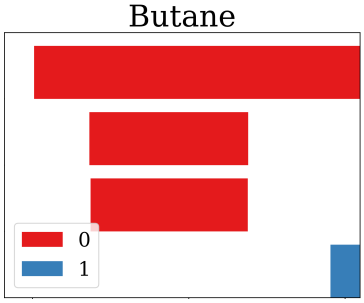
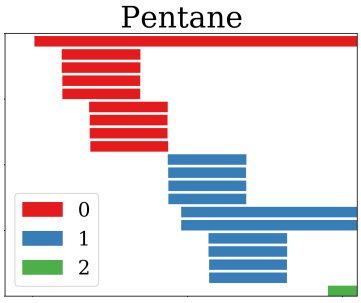
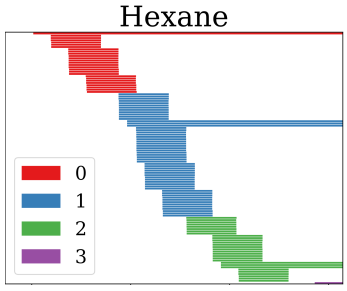
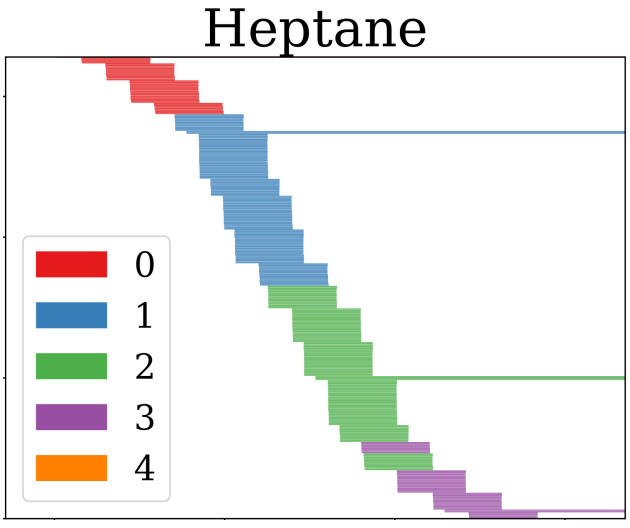
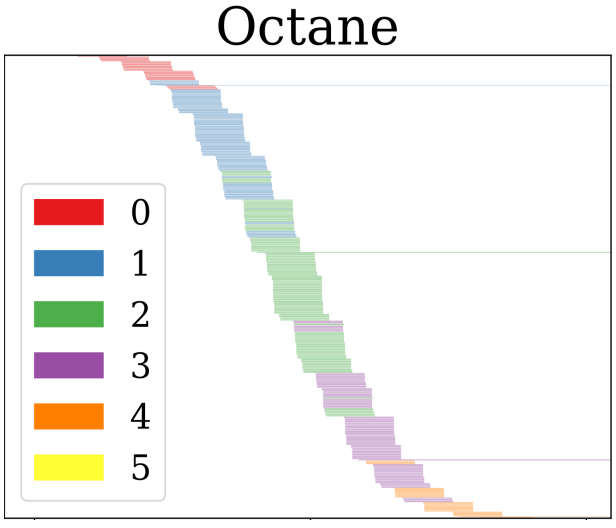










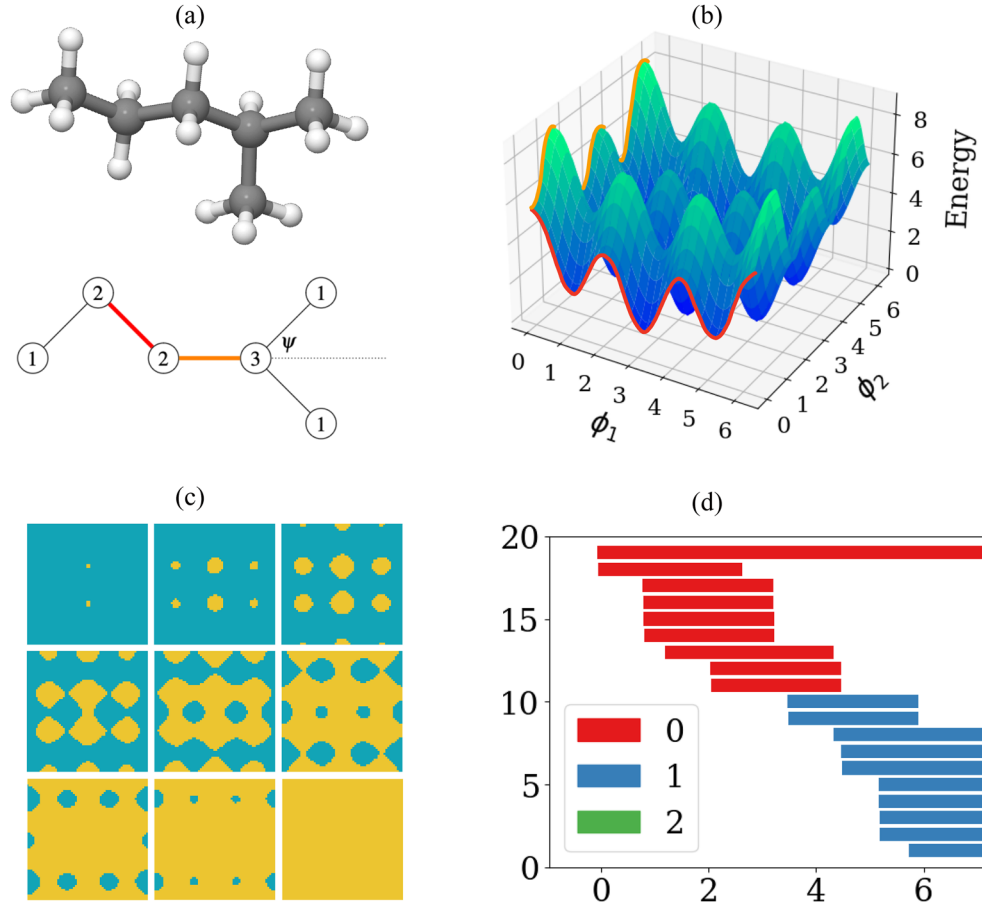
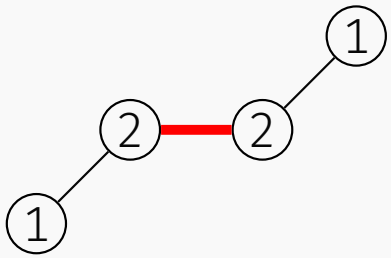


FIG. 1. (a) Covalent bond graph of 2-methyl pentane with the degree of each C-atom listed. The dotted line is the angle bisector between the two leaf carbons, and ψ denotes the angle between the bisector and the leaf carbons. (b) The potential energy landscape (PEL) of 2-methyl pentane (in kcal/mol), where the orange curve is the PEL of isopentane and the red curve is the PEL of butane. The variables ϕ_1 and ϕ_2 correspond to the dihedral angles of butane and isopentane, respectively. (c) Nine sublevelsets of the 2-methyl pentane PEL (yellow) with energy values in kcal/mol of 0, 1.041, 2.082, 3.123, 4.164, 5.206, 6.247, 7.288, and 12.493. The zero of energy represents the global minimum. (d) Sublevelset persistence barcode for the 2-methyl pentane PEL. The *x*-axis denotes the energy value (in kcal/mol), and the *y*-axis gives the total number of bars. The color denotes the topological dimension of the bar. Semi-infinite bars extend to the end of the energy scale.

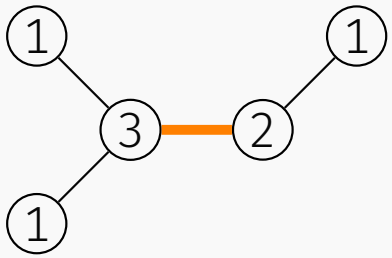
Additive functions on a product space

Definition 2

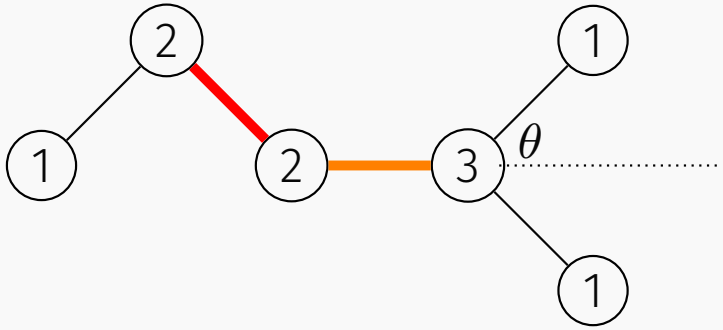
If $g_i : X_i \to \mathbb{R}$ is a collection of functions for $i = 1, \ldots, n$, then one can define their sum f on the product space by $f\colon X_1 \times \ldots \times X_n \to \mathbb{R}$ given by $f(x_1, \ldots, x_n) = g_1(x_1) + \ldots + g_n(x_n)$.



$g_1 : S^1 \to \mathbb{R}$



$g_2 : S^1 \to \mathbb{R}$

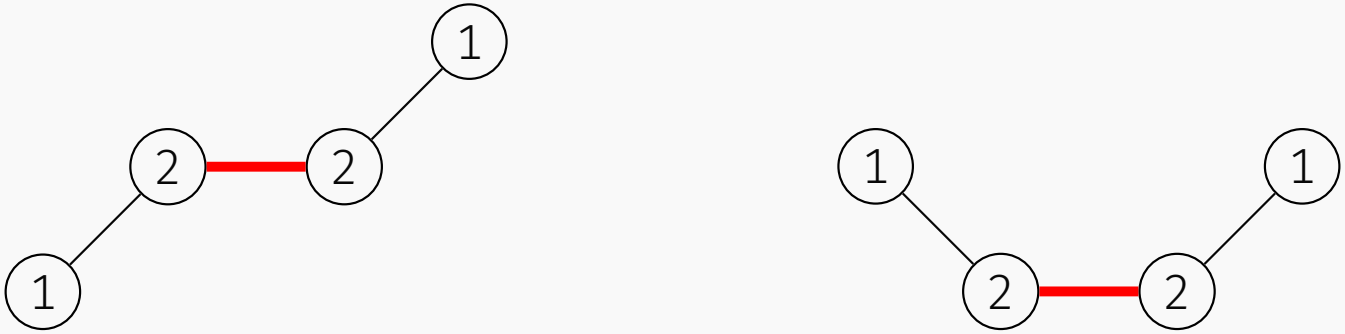


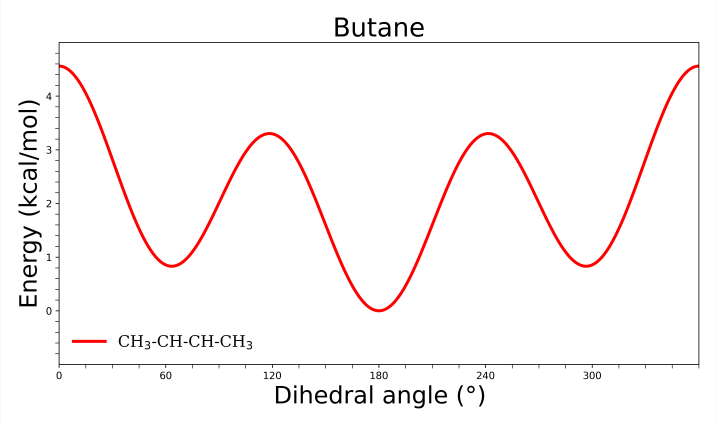
$f\colon (S^1)^2 \to \mathbb{R}$

$$f(\phi_1, \phi_2) = g_1(\phi_1) + g_2(\phi_2)$$

Energy landscapes

What is an Optimized Potentials for Liquid Simulations - United Atom (OPLS-UA) energy landscape?

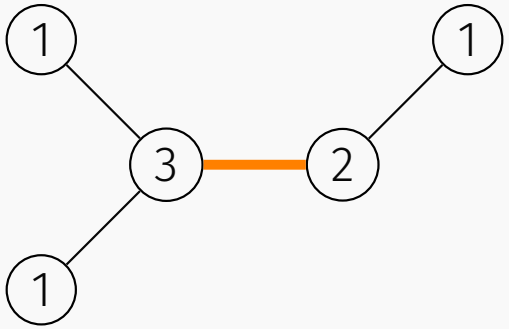


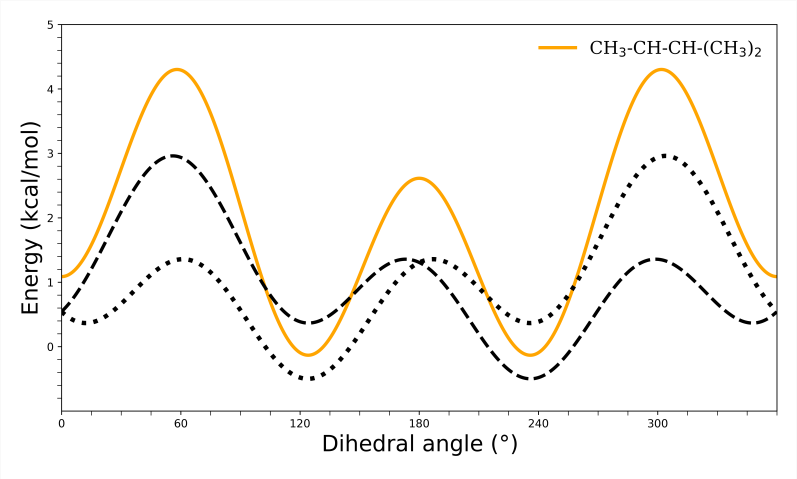


$$V_{1\text{-}2\text{-}2\text{-}1}(\phi_1) = c_0 + c_1[1 + \cos(\phi_1)] + c_2[1 - \cos(2\phi_1)] + c_3[1 + \cos(3\phi_1)]$$

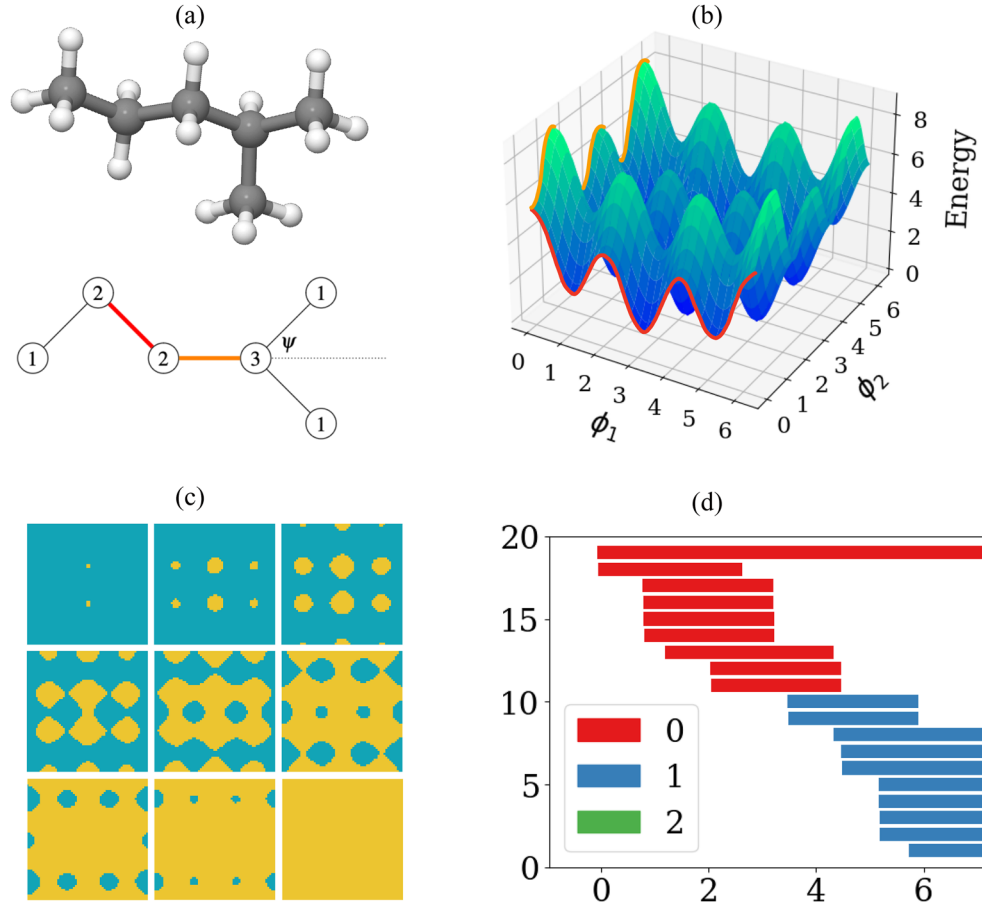
Energy landscapes

What is a branched alkane?





$$f(\phi_1) = \mathrm{V}_{\text{1-3-2-1}}(\phi_2 + \theta) + \mathrm{V}_{\text{1-3-2-1}}(\phi_2 - \theta)$$



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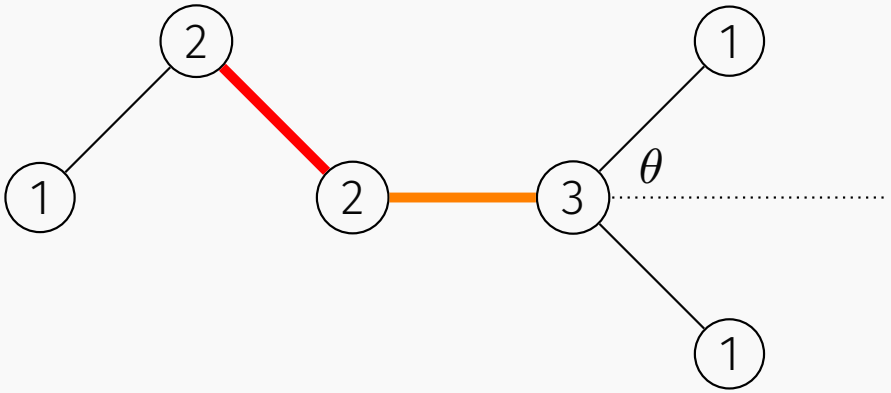
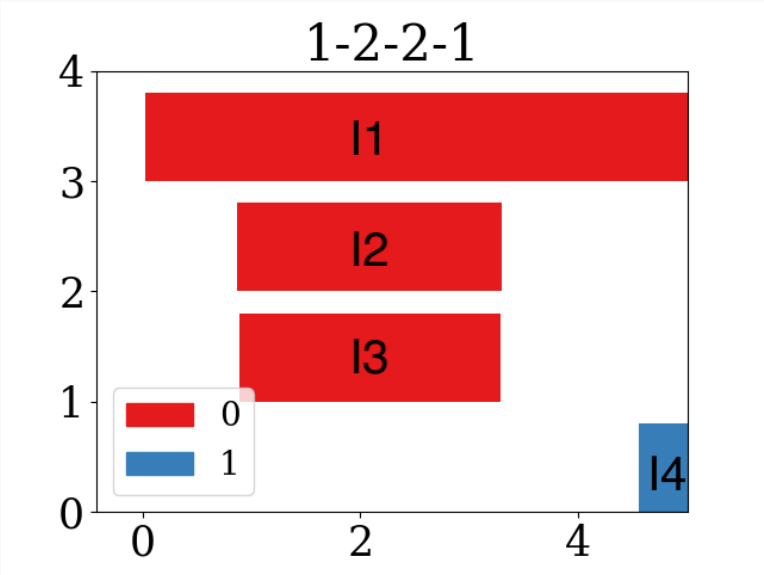
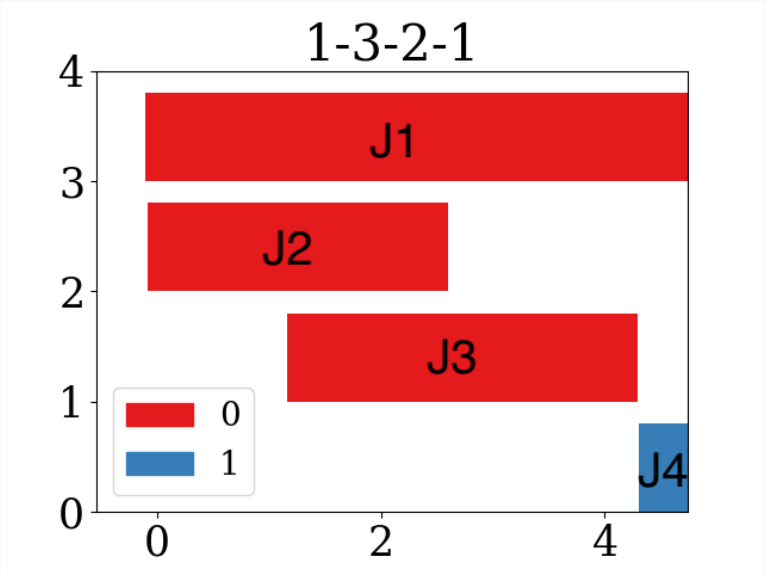
2,2-METHYLPENTANE







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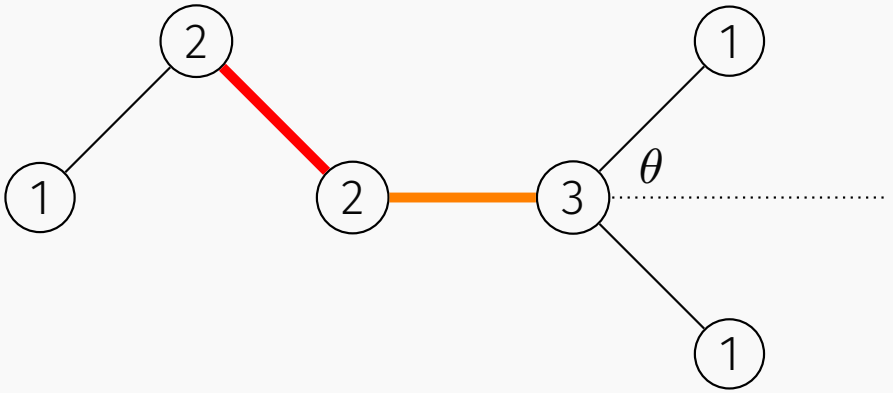
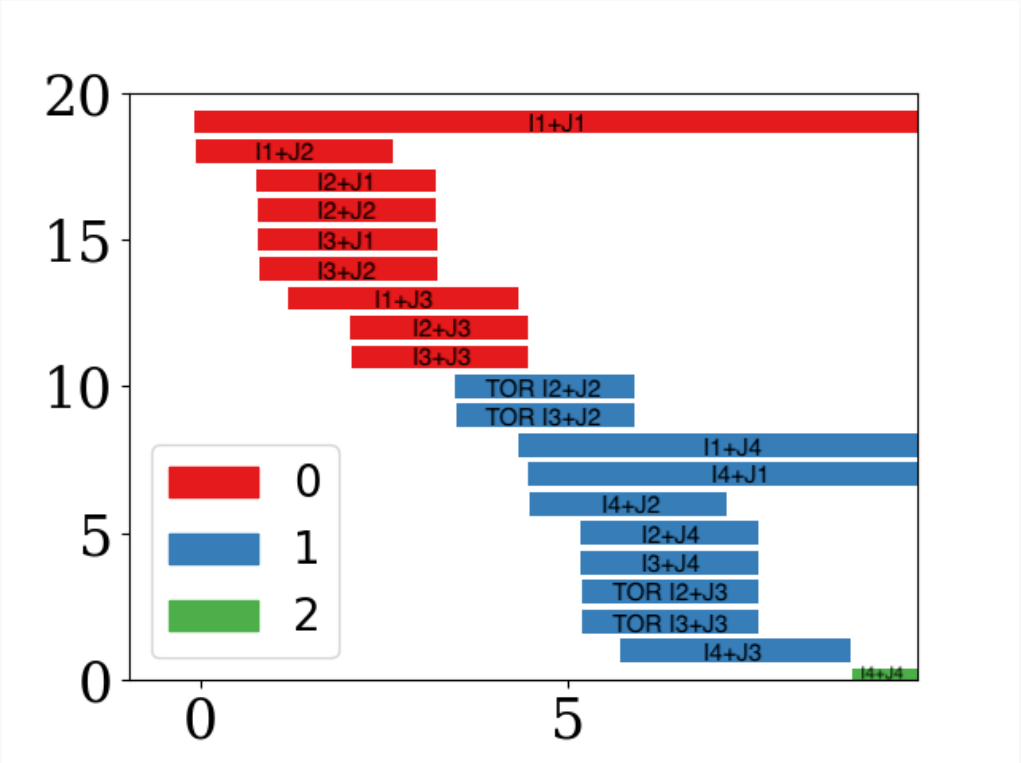




Künneth Formula

Theorem 4 (Persistent Künneth Formula [GP19])

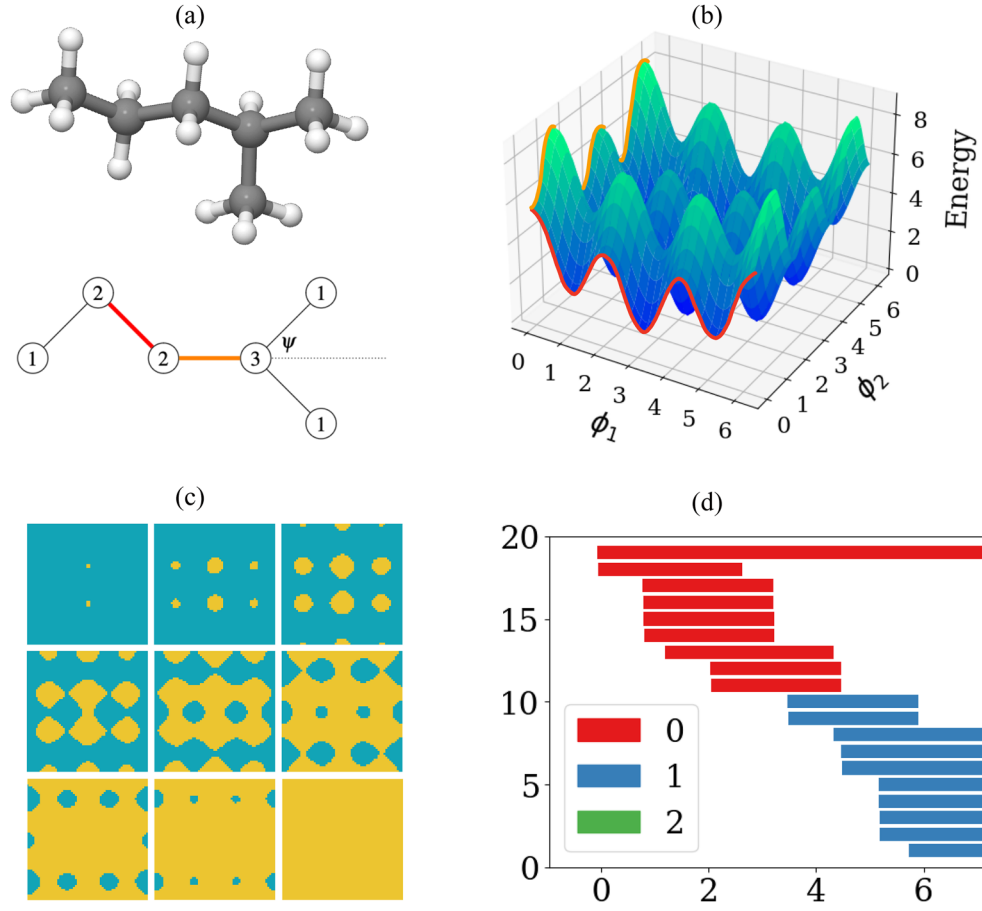
There is a natural short exact sequence of graded modules

$$0 \to \bigoplus_{i+j=n} (PH_i(X) \otimes PH_j(Y)) \to PH_n(X \otimes_f Y) \to \bigoplus_{i+j=n} \mathrm{Tor}(PH_i(X), PH_{j-1}(Y)) \to 0.$$

If $H_i(X)$ and $H_j(Y)$ are point-wise finite, then

$$\begin{aligned}
&\mathrm{bcd}_n(X \otimes_f Y) \\
&= \bigsqcup_{i+j=n} \left\{ (\ell_J + I) \cap (\ell_I + J) \mid I \in \mathrm{bcd}_i(X), J \in \mathrm{bcd}_j(Y) \right\} \\
&\quad \sqcup \bigsqcup_{i+j=n} \left\{ (r_J + I) \cap (r_I + J) \mid I \in \mathrm{bcd}_i(X), J \in \mathrm{bcd}_{j-1}(Y) \right\} \\
&= \bigsqcup_{i+j=n} \left\{ [\ell_I + \ell_J, \mathsf{min}(\ell_J + r_I, \ell_I + r_J)) \mid I \in \mathrm{bcd}_i(X), J \in \mathrm{bcd}_j(Y) \right\} \\
&\quad \sqcup \bigsqcup_{i+j=n} \left\{ [\mathsf{max}(\ell_I + r_J, \ell_J + r_I), r_I + r_J) \mid I \in \mathrm{bcd}_i(X), J \in \mathrm{bcd}_{j-1}(Y) \right\}.
\end{aligned}$$

Here ℓ and r are the left and right endpoints of the interval.



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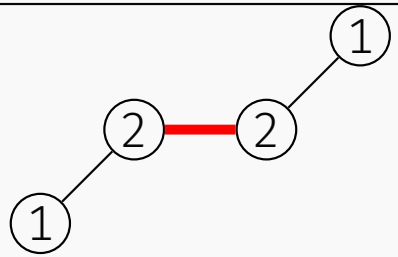
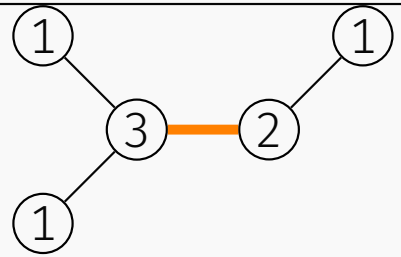
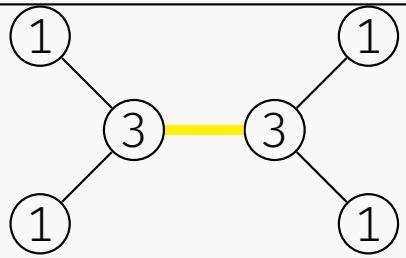
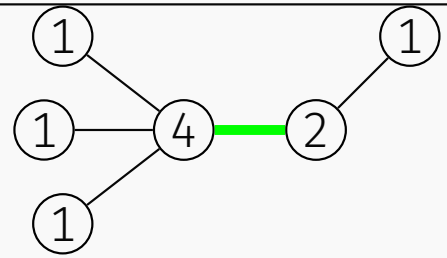
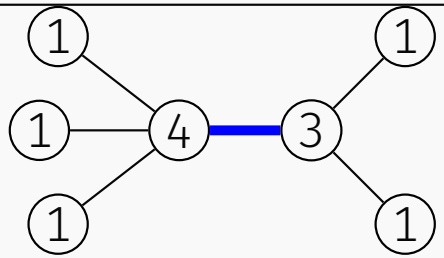
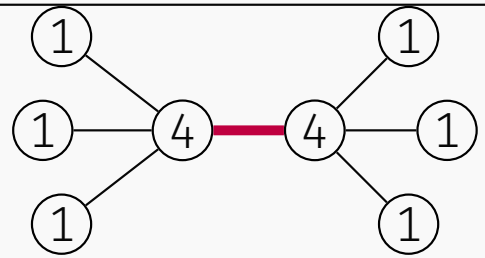
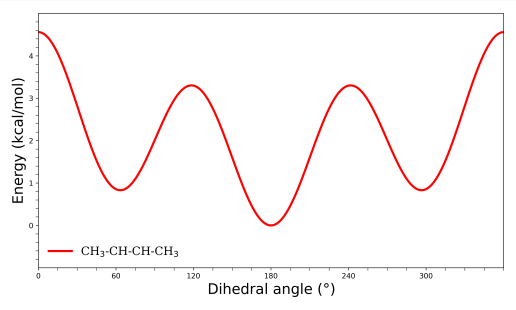
Internal Base Bond Types

1-2-2-1: butane	1-3-2-1: isopentane
	
1-3-3-1: 2,3-dimethylbutane	1-4-2-1: 2,2-dimethylbutane
	
1-4-3-1: triptane	1-4-4-1: tetramethylbutane
	

EL's and sublevelset persistence of base bonds

1-2-2-1



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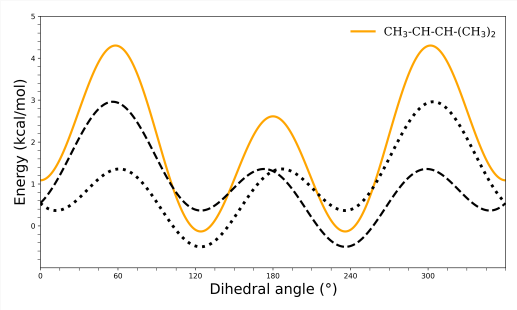
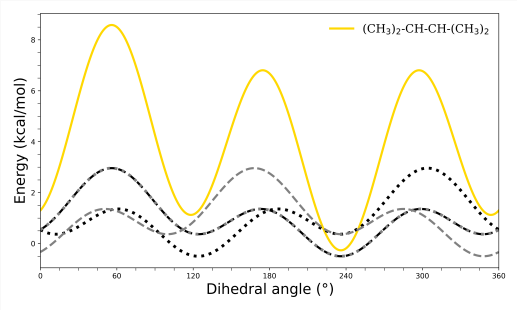
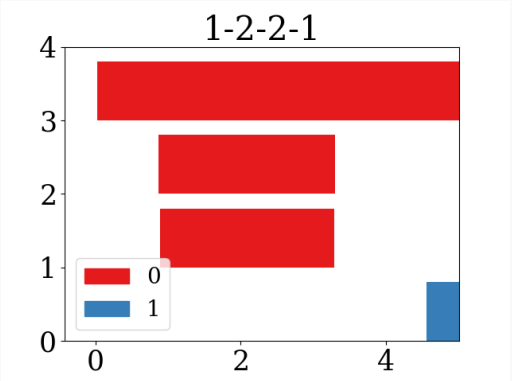
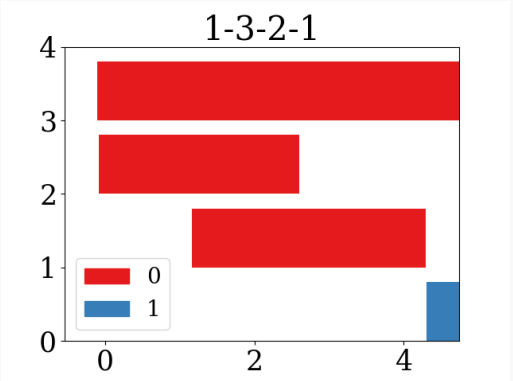
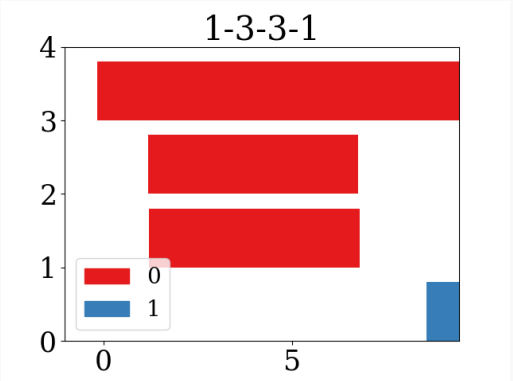


1-3-3-1



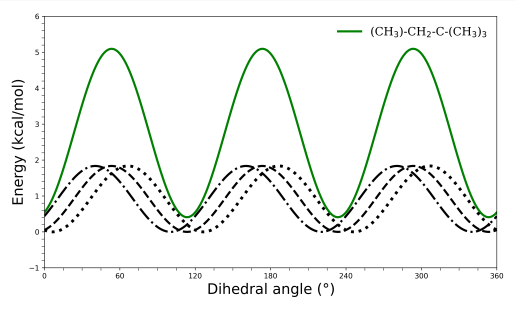




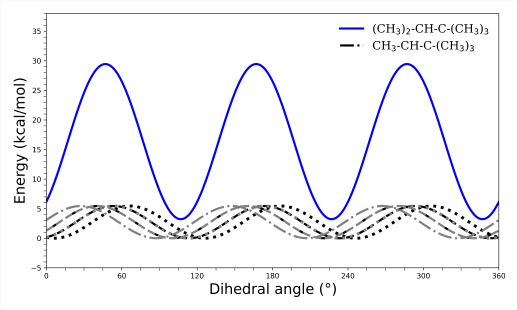


EL's and sublevelset persistence of base bonds

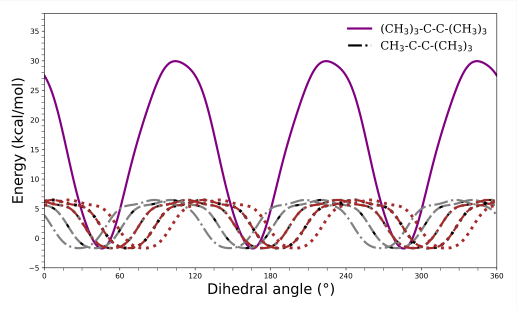
1-4-2-1

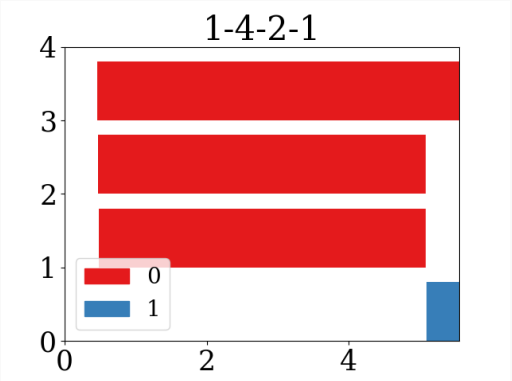


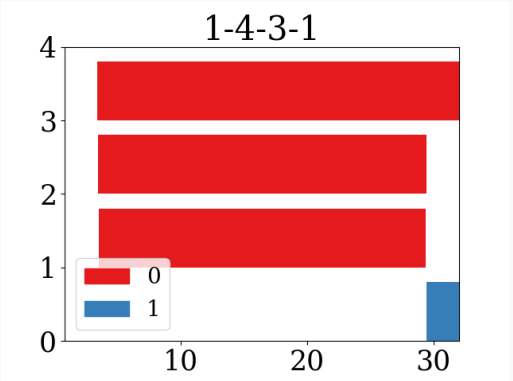
1-4-3-1

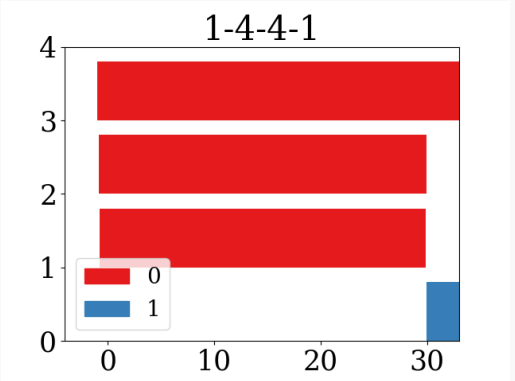


1-4-4-1

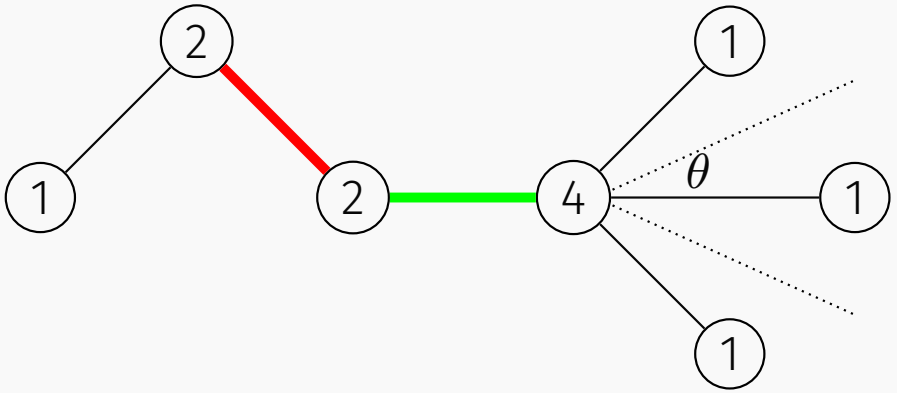


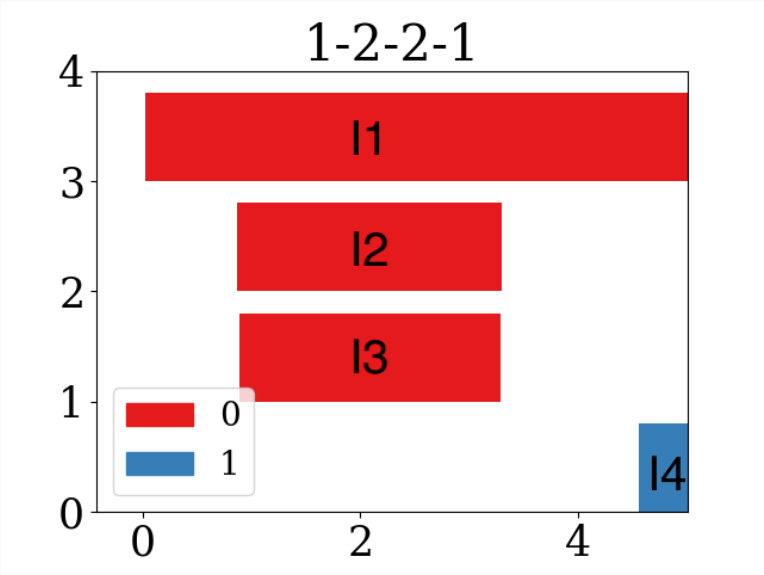


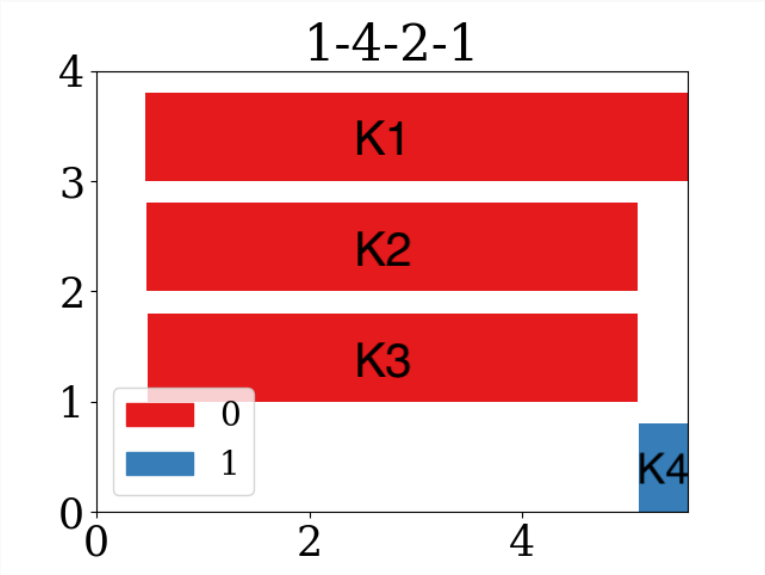




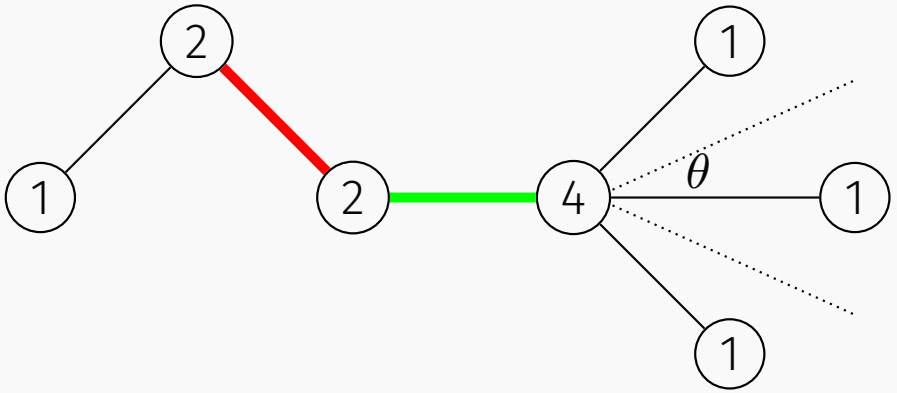
2,2-DIMETHYLPENTANE

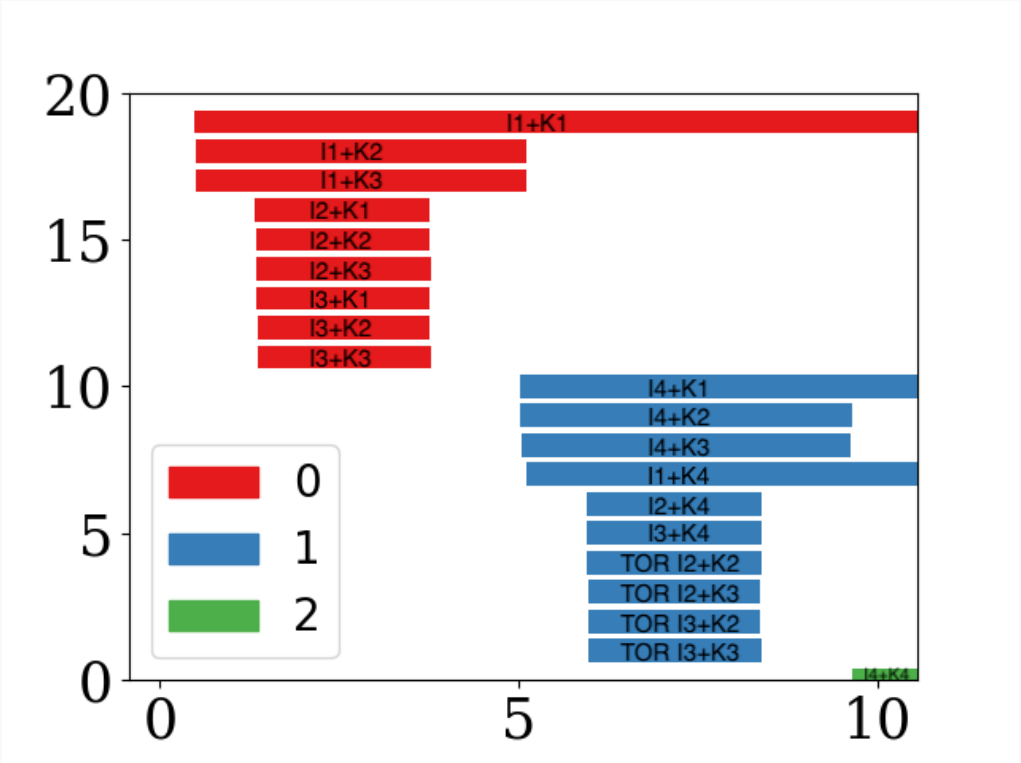






2,2-DIMETHYLPENTANE





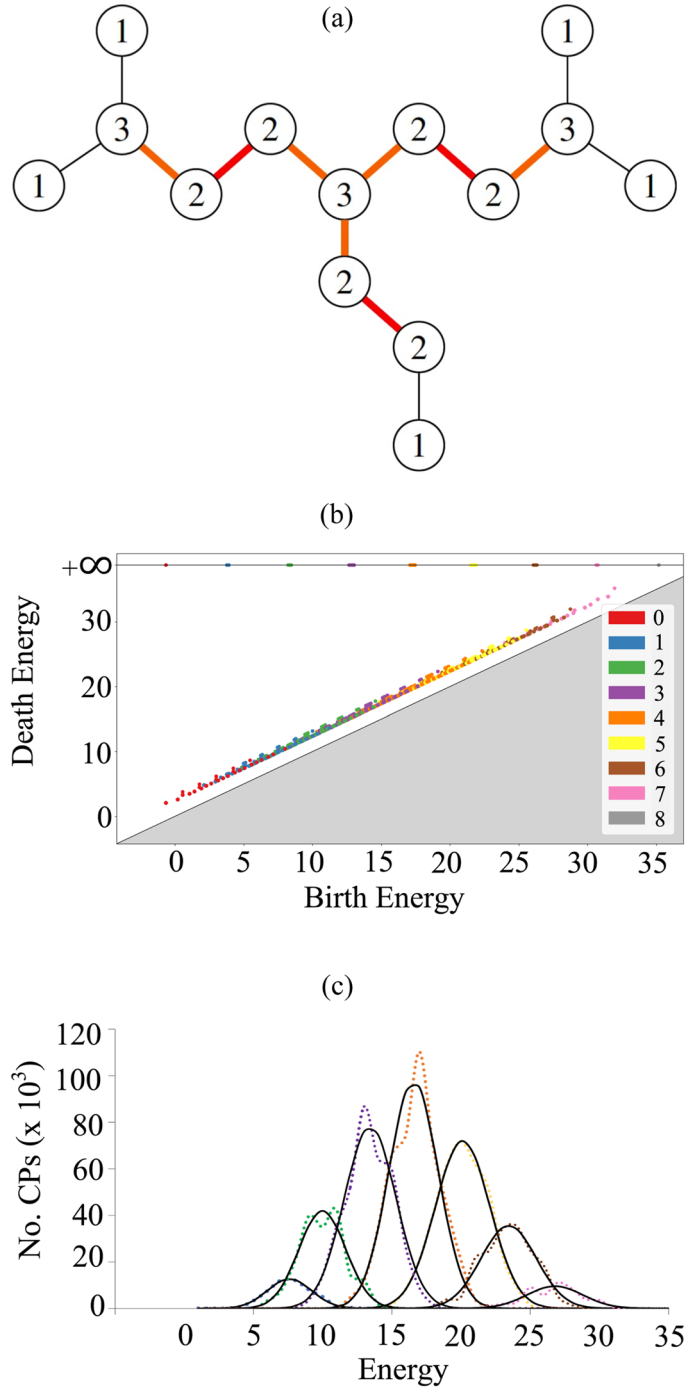


FIG. 7. (a) 2,8-dimethyl, 5-propyl nonane consists of five 1-3-2-1 building blocks and three 1-2-2-1 building blocks. (b) The persistence diagram. Each dot represents a set of bars on the persistence barcode with the same birth and death times. The *x*-axis is the energy value of the bar's birth and the *y*-axis is the energy value of the bar's death, both in (kcal/mol). (c) The number of critical points (CPs) of each index as a function of energy (kcal/mol); each index has the same color as the corresponding topological dimension.

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