

Berger–Gritzmann–de Vries Cycle Invariants

Worked Examples for Small Molecular Graph Models

Algorithmic Cheminformatics, 2026

Berger’s invariant, in the notation used here

We follow the terminology from Berger, Gritzmann, and de Vries, *Minimum Cycle Bases and Their Applications*, Section 3.2. All edge weights in the examples below are one unless stated otherwise. Cycle sums and linear independence are taken over $\text{GF}(2)$, so adding two cycles means taking the symmetric difference of their edge sets.

For a connected graph $G = (V, E)$, the dimension of the cycle space is

$$\mu(G) = |E| - |V| + 1.$$

A minimum cycle basis (MCB) is a cycle basis $B = \{C_1, \dots, C_\mu\}$ of minimum total weight. The sorted weight vector

$$\vec{w}(G) = (w(C_1), \dots, w(C_\mu))$$

is already a graph invariant, but it only records the lengths/weights of the selected basis cycles.

Berger et al. refine this by using interchangeability classes. Fix a cycle weight κ . Relevant cycles of weight κ are partitioned into equivalence classes W^κ , also called interchangeability classes. The important number attached to such a class is not only its cardinality $|W^\kappa|$, but its relative rank

$$r(W^\kappa) = |B \cap W^\kappa|,$$

where B is any MCB. Berger et al. show that this number is independent of the chosen MCB.

We use the compact encoding from the paper: vertical bars separate interchangeability classes, the entries are the weights contributed by an MCB, and a subscript e means that the corresponding interchangeability class has cardinality one. For example,

$$(|6_e|6_e|6_e|)$$

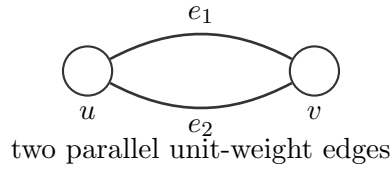
means three singleton classes of hexagons, each of relative rank one, whereas

$$(|6, 6, 6|)$$

means one class of hexagons with relative rank three. The latter class may contain more than three cycles; an MCB takes three of them.

Modeling note. Berger’s cycle invariant is applied here to the graph model that is explicitly drawn. The graph model matters. The first two examples deliberately use multigraphs to show what happens for parallel edges. The aromatic examples later are Kekulé multigraphs: a drawn double bond is counted as two parallel unit-weight graph edges. No aromatic-circle edges are used. Thus the invariant describes the chosen Kekulé graph model, not an aromatic bond-order abstraction.

1 Two vertices with two parallel edges: a double-bond multi-graph



Here $|V| = 2$, $|E| = 2$, hence

$$\mu(G) = 2 - 2 + 1 = 1.$$

The only cycle is the 2-cycle

$$C_{12} = \{e_1, e_2\}.$$

It has weight 2, and the unique MCB is

$$B = \{C_{12}\}.$$

Thus

$$\vec{w}(G) = (2).$$

There is exactly one relevant cycle of weight 2, hence exactly one \sim_2 -class:

$$W^2 = \{C_{12}\}, \quad |W^2| = 1, \quad r(W^2) = 1.$$

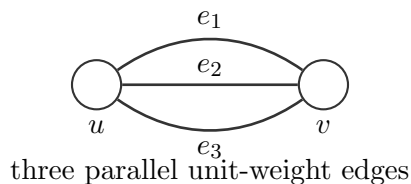
class	relevant cycles in the class	relative rank
W_1^2	$\{C_{12}\}$	1

The Berger encoding is therefore

$$\boxed{(|2_e|)}.$$

The subscript e records that the class has cardinality one.

2 Two vertices with three parallel edges: a triple-bond multi-graph



Now $|V| = 2$, $|E| = 3$, and

$$\mu(G) = 3 - 2 + 1 = 2.$$

There are three 2-cycles:

$$C_{12} = \{e_1, e_2\}, \quad C_{13} = \{e_1, e_3\}, \quad C_{23} = \{e_2, e_3\}.$$

They satisfy one GF(2)-relation:

$$C_{12} \oplus C_{13} \oplus C_{23} = 0.$$

Equivalently, any one of them is the sum of the other two. Hence any two of the three cycles form a minimum cycle basis:

$$\{C_{12}, C_{13}\}, \quad \{C_{12}, C_{23}\}, \quad \{C_{13}, C_{23}\}.$$

Every MCB has two cycles of weight 2, so

$$\vec{w}(G) = (2, 2).$$

All three relevant 2-cycles have the same function in an MCB: one may exchange one for another and still obtain an MCB. Thus there is one interchangeability class

$$W^2 = \{C_{12}, C_{13}, C_{23}\}, \quad |W^2| = 3, \quad r(W^2) = 2.$$

one class $W^2 = \{C_{12}, C_{13}, C_{23}\}$; every MCB chooses exactly two cycles from it.

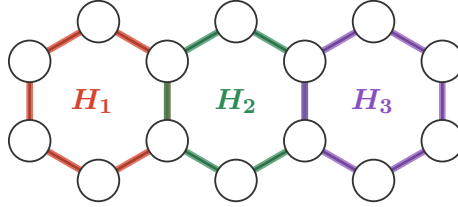
The Berger encoding is

$$\boxed{(|2, 2|)}.$$

There is no subscript e , because the class has cardinality 3, not 1.

3 Three 6-cycles in a row

This is the unweighted graph obtained from three hexagons fused linearly. It is a schematic model for a chain of three six-membered rings.



The graph has $\mu = 3$. The three hexagons

$$H_1, \quad H_2, \quad H_3$$

have weight 6 and form a cycle basis. The larger cycles obtained by combining adjacent hexagons have weights 10 and 10, and the outer cycle around all three hexagons has weight 14. Thus an MCB is forced to use exactly the three hexagons:

$$B = \{H_1, H_2, H_3\}, \quad \vec{w}(G) = (6, 6, 6).$$

Each hexagon is unique in its role. For instance, H_1 is the only relevant cycle of weight 6 containing the leftmost outer edges; analogous statements hold for H_2 and H_3 . Consequently, the three hexagons define three singleton interchangeability classes:

$$W_1^6 = \{H_1\}, \quad W_2^6 = \{H_2\}, \quad W_3^6 = \{H_3\}.$$

Each has cardinality 1 and relative rank 1.

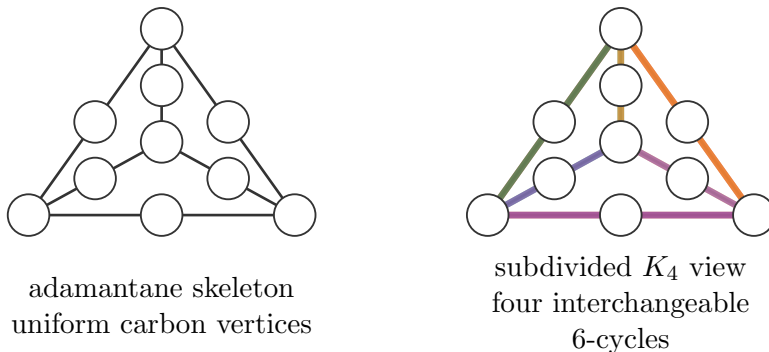
class	cardinality	relative rank
$W_1^6 = \{H_1\}$	1	1
$W_2^6 = \{H_2\}$	1	1
$W_3^6 = \{H_3\}$	1	1

The Berger encoding is

$$\boxed{(|6_e|6_e|6_e|)}.$$

4 Adamantane: four interchangeable hexagons

Adamantane's carbon skeleton is conveniently viewed as a subdivision of K_4 : the four degree-three carbon atoms play the role of the vertices of K_4 , and each edge of K_4 is subdivided once. The four triangles of K_4 become four 6-cycles in the subdivided graph.



Here $|V| = 10$, $|E| = 12$, hence

$$\mu(G) = 12 - 10 + 1 = 3.$$

The four 6-cycles satisfy

$$H_1 \oplus H_2 \oplus H_3 \oplus H_4 = 0.$$

Therefore any three of them form a minimum cycle basis:

$$\{H_1, H_2, H_3\}, \quad \{H_1, H_2, H_4\}, \quad \{H_1, H_3, H_4\}, \quad \{H_2, H_3, H_4\}.$$

All MCBs have the same weight vector

$$\vec{w}(G) = (6, 6, 6).$$

Unlike the linear chain of three hexagons, these four hexagons are interchangeable. There is a single \sim_6 -class

$$W^6 = \{H_1, H_2, H_3, H_4\}, \quad |W^6| = 4, \quad r(W^6) = 3.$$

The relative rank is 3, because every MCB contains three cycles from this class.

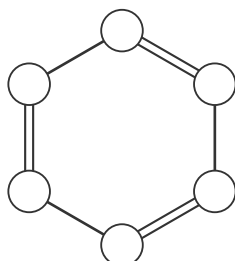
The Berger encoding is

$$\boxed{(|6, 6, 6|)}.$$

This is exactly the distinction emphasized in Berger et al.'s Fig. 3: the plain vector $(6, 6, 6)$ is the same as for three unique hexagons, but the interchangeability structure is different.

5 One Kekulé benzene ring

We draw one Kekulé structure of benzene. For this example, each drawn double bond is counted as two parallel unit-weight graph edges. No aromatic-circle edge is used.



one Kekulé multigraph model of benzene
each double bond contributes a parallel edge

The graph has $|V| = 6$ and $|E| = 9$, because the three double bonds contribute one additional parallel edge each. Hence

$$\mu(G) = 9 - 6 + 1 = 4.$$

The three double bonds give three local 2-cycles:

$$D_{12}, \quad D_{34}, \quad D_{56}.$$

Each of these 2-cycles is forced into every MCB, because it is the unique way to represent the corresponding parallel-edge direction in the cycle space.

After that, one 6-cycle around the ring is needed. There are $2^3 = 8$ such 6-cycles: for each of the three double bonds one may choose either of its two parallel edges. They are interchangeable; an MCB takes one representative from this family. Thus

$$B = \{D_{12}, D_{34}, D_{56}, H\}, \quad \vec{w}(G) = (2, 2, 2, 6).$$

The interchangeability classes are

$$W_1^2 = \{D_{12}\}, \quad W_2^2 = \{D_{34}\}, \quad W_3^2 = \{D_{56}\},$$

all of cardinality 1 and relative rank 1. Let W^6 denote the family of the eight 6-cycles obtained by choosing one edge from each double bond. Then

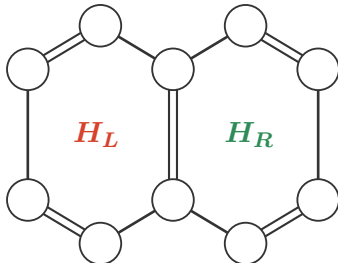
$$|W^6| = 8, \quad r(W^6) = 1.$$

The Berger encoding is

$$\boxed{(|2_e|2_e|2_e|6|)}.$$

6 Two fused Kekulé rings

Here the two aromatic rings are fused, not bridged. The drawing shows one Kekulé structure, with the fused edge drawn as a double bond. For this example, every drawn double bond is counted as two parallel unit-weight graph edges. Again, no aromatic-circle edge is used.



one fused-edge Kekulé multigraph model of naphthalene
each double bond contributes a parallel edge

The simple fused skeleton has 11 edges. The chosen Kekulé drawing has five double bonds, so the multigraph has $|V| = 10$ and $|E| = 16$. Hence

$$\mu(G) = 16 - 10 + 1 = 7.$$

The five double bonds give five forced local 2-cycles:

$$D_{12}, \quad D_{34}, \quad D_{56}, \quad D_{78}, \quad D_{9,10}.$$

The remaining two basis directions are represented by a left and a right hexagon. For the left hexagon there are $2^3 = 8$ variants, because it contains the double bonds 12, 34, and 56. For the right hexagon there are also $2^3 = 8$ variants, because it contains the double bonds 34, 78, and 9,10. An MCB contains all five 2-cycles, one left hexagon, and one right hexagon:

$$B = \{D_{12}, D_{34}, D_{56}, D_{78}, D_{9,10}, H_L, H_R\}.$$

Hence

$$\vec{w}(G) = (2, 2, 2, 2, 2, 6, 6).$$

The 2-cycle classes are singleton classes, each of relative rank 1. The left and right hexagon families are distinct interchangeability classes:

$$|W_L^6| = 8, \quad r(W_L^6) = 1, \quad |W_R^6| = 8, \quad r(W_R^6) = 1.$$

The Berger encoding is

$$\boxed{(|2_e|2_e|2_e|2_e|2_e|6|6|)}.$$

Dependence on the chosen Kekulé structure. This is a graph invariant of the chosen Kekulé multigraph. For naphthalene there are Kekulé structures with and without the fused edge as a double bond. Changing that choice changes the multigraph, and may therefore change the cycle invariant.

Summary

graph model	$\mu(G)$	$\vec{w}(G)$	Berger encoding
two parallel edges	1	(2)	(2 _e)
three parallel edges	2	(2, 2)	(2, 2)
three fused hexagons in a row	3	(6, 6, 6)	(6 _e 6 _e 6 _e)
adamantane skeleton	3	(6, 6, 6)	(6, 6, 6)
one Kekulé benzene ring	4	(2, 2, 2, 6)	(2 _e 2 _e 2 _e 6)
two fused Kekulé rings	7	(2, 2, 2, 2, 2, 6, 6)	(2 _e 2 _e 2 _e 2 _e 2 _e 6 6)

The key pedagogical contrast is the pair

$$(|6_e|6_e|6_e|) \quad \text{versus} \quad (|6, 6, 6|).$$

Both have the same MCB weight vector (6, 6, 6), but the first describes three forced singleton hexagons, while the second describes one interchangeable family of four hexagons from which every MCB takes three.