

**Exercise 1:**

Let  $P_1$  and  $P_2$  be two permutation matrices. Is  $P_1 \times P_2$  also a permutation matrix? Argue for or against your answer.

**Exercise 2:**

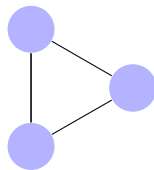
1. Draw the graphs  $G_A$  and  $G_B$  for which the following 2 adjacency matrices  $A$  and  $B$  are given.

$$A = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix} \quad B = \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}$$

2. Are the two graphs isomorphic?
3. How many different representations (in terms of adjacency matrices) of  $G_A$  are there?
4. How many different representations (in terms of adjacency matrices) of  $G_B$  are there?
5. Is there a permutation matrix  $P$  such that  $A = P(PB)^T$  holds?
6. If so, give all matrices  $P$ , such that  $A = P(PB)^T$  holds.

**Exercise 3:**

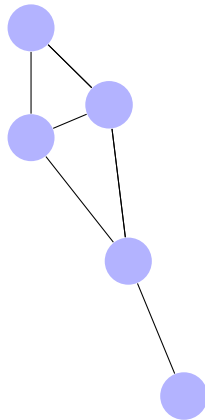
Given the following graph:



1. Give an adjacency matrix  $A$  for the graph. (How many different are there?)
2. For your chosen adjacency matrix, how many permutation matrices  $P$  are there, such that  $A = P(PA)^T$  holds? (Remark: this number corresponds to the size of the so-called “automorphism group” of the graph).

**Exercise 4:**

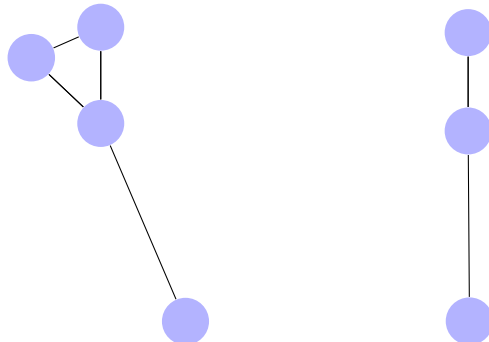
Given the following graph:



1. Give an adjacency matrix  $A$  for the graph.
2. For your chosen adjacency matrix, how many permutation matrices  $P$  are there, such that  $A = P(PA)^T$  holds?

**Exercise 5\*:**

Given the following two graphs  $G_A$  (left) and  $G_B$  (right):



1. Give adjacency matrices for  $G_A$  and  $G_B$ .
2. Is  $G_B$  a subgraph of  $G_A$ ?
3. How many different ways are there to find  $G_B$  as a subgraph in  $G_A$ ? (i.e., assuming as adjacency matrix  $A$  and  $B$  for graphs  $G_A$  and  $G_B$ , how many leaf-nodes would the search tree of the Ullmann algorithm have?)

4. How many different ways are there to find  $G_B$  as an induced subgraph in  $G_A$ ?

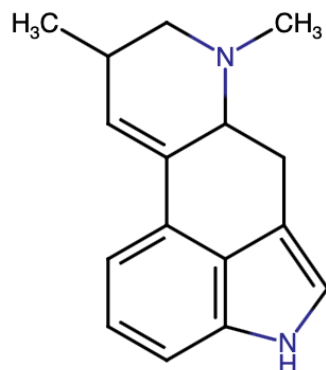
**Exercise 6:**

The following is from the unit-testing of the graph theory assignment. Explain the expected result 10.

```
>>> A = np.array([[ 0,  1,  0,  0,  1], \
                  [ 1,  0,  1,  0,  0], \
                  [ 0,  1,  0,  1,  0], \
                  [ 0,  0,  1,  0,  1], \
                  [ 1,  0,  0,  1,  0]])
>>> numIsomorphisms(A, A)
10
```

**Exercise 7\*:**

Use sigma aldrich <https://www.sigmaaldrich.com/DK/en/structure-search> to look for chemical structures. How many structures can you find which have the following as a substructure?



Can you find the price for the compound(s) you found? Do you know the compound with the highest similarity?