ECM32 – XXXII European Crystallographic Meeting

MaThCryst Satellite Meeting

Graph Theory and Modular Structures

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Bernd Souvignier

Radboud University Nijmegen

Graph Theory in Crystal Structure Description

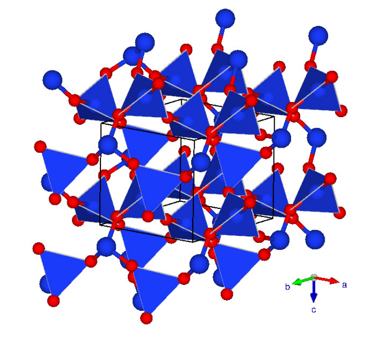
Overview

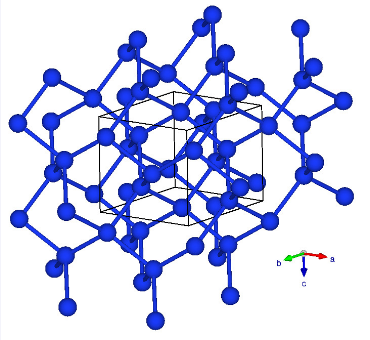
- historical review
- basic concepts
- algebraic description
- quotient graphs
- voltage graphs
- embeddings

From crystal structures to graphs

Representation of crystal structures

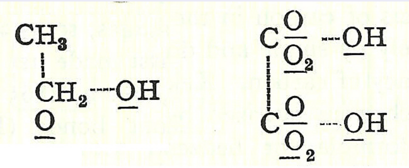
Crystal structures are represented graphically in various ways, e.g. by coordination polyhedra or ball-and-stick models, showing not only the atoms, but also the bonds between them.



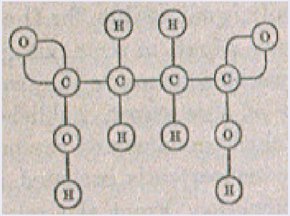


Abstraction from the concrete atoms leads to the mathematical concept of graphs, consisting of vertices and edges displaying adjacency between certain vertices.

Some early examples



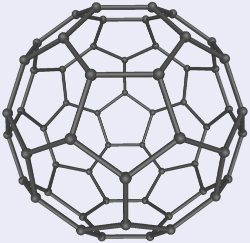
Archibald Scott Couper (1858)

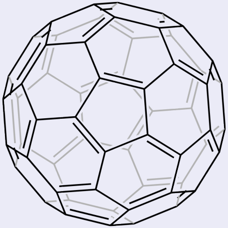


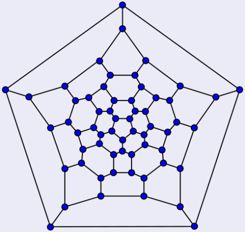
Alexander Crum Brown (1864)

The term graph was introduced in 1878 by James Joseph Sylvester.

Different representations of fullerenes

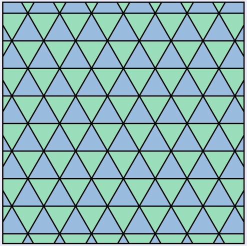
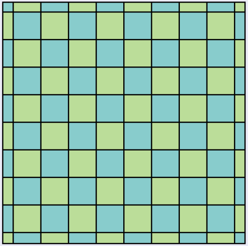
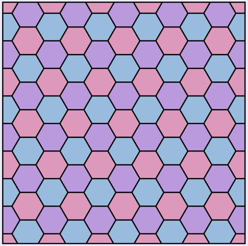




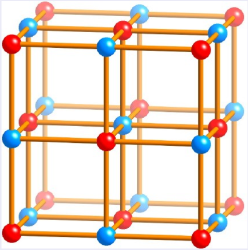
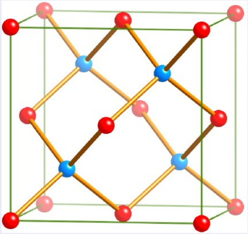
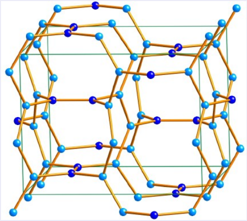


2- and 3-dimensional nets

2-dimensional regular tilings

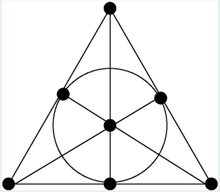




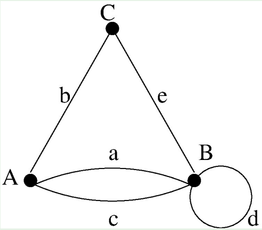
Examples of 3-dimensional periodic nets

Definition

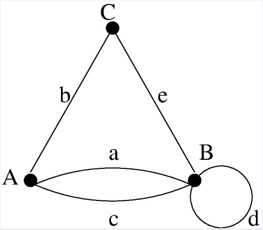
- A graph $\mathcal{G}$ consists of a vertex set $\mathcal{V} = \mathcal{V}(\mathcal{G})$ and an edge set $\mathcal{E} = \mathcal{E}(\mathcal{G})$, where each edge $e \in \mathcal{E}$ has assigned to it its endpoints $X, Y \in \mathcal{V}$.





- A simple graph is a graph without multiple edges and without loops, i.e. each pair of vertices is connected by at most one edge and the two endpoints of each edge are distinct.
- To stress that a graph may contain multiple edges or loops it is sometimes called a multigraph.
- The vertices and edges of a graph may or may not carry labels.

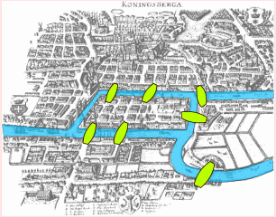
Some terminology

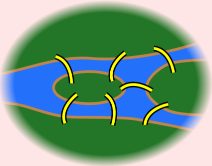


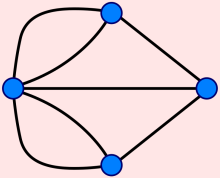
- The number $n = \#\mathcal{V}$ of vertices of a graph is called its order, the number $m = \#\mathcal{E}$ of edges its size.
- The number of edges emerging from a vertex X is called the degree of X, denoted by $\deg X$. A loop at X contributes 2 to $\deg X$.
  Example: $\deg A = 3$, $\deg B = 5$, $\deg C = 2$
- Two vertices are called adjacent or neighbours, if they are connected by an edge.
- Two edges are called adjacent if they share a vertex.
- The endpoints of an edge are said to be incident with that edge.

Exercise: The seven bridges of Königsberg (1736)

- Is there a route around the city of Königsberg which crosses each of the seven bridges across the river Pregel precisely once?







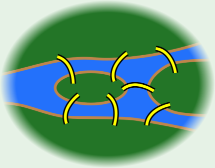
Such a route is called an Euler walk – or an Euler circuit in case it is a closed walk.

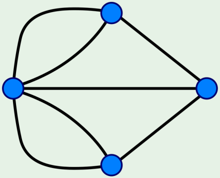
- Is there an Euler walk if one bridge is omitted?
- And with one bridge extra?
- How many extra bridges are required (and where) to obtain an Euler circuit?

Solution: The seven bridges of Königsberg

There exists an Euler circuit if and only if all vertices have even degree.

There exists an Euler walk that is not a circuit if and only if there are precisely two vertices with odd degree. In this case, these are the initial and terminal vertices of the walk.

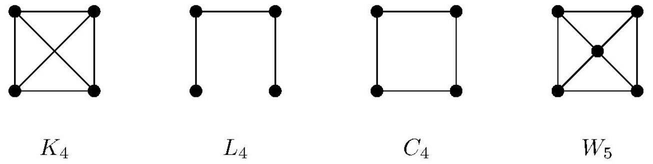




Since all vertices have odd degree, omitting or adding one bridge allows for an Euler walk.

Introducing two extra bridges between disjoint pairs of vertices allows for an Euler circuit.

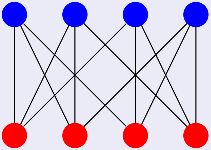
Some standard types of simple graphs

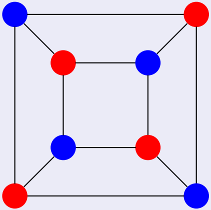


- In the complete graph K_n of order n, every pair of distinct vertices is connected by a single edge. The size of K_n is $n(n-1)/2$.
- In the linear graph L_n of order n, the vertices are arranged in a line. The size of L_n is $n-1$.
- The cycle graph C_n of order n is obtained by connecting the two endpoints of the linear graph L_n. Thus, in the cycle graph, every vertex has exactly two neighbours. The size of C_n is n.
- The wheel graph W_n of order n consists of a cycle graph of order $n-1$ and an additional vertex which is connected to every vertex of the cycle graph by a single edge. The size of W_n is $2n-2$.

Bipartite graphs

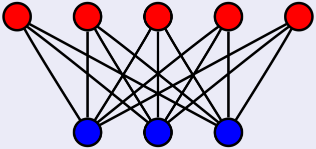
In a bipartite graph, the vertices can be coloured with two colours such that only vertices of different colour are adjacent.





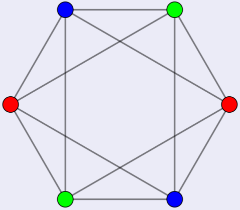
The complete bipartite graph $K_{n,m}$ contains all edges between pairs of vertices of different colour.

$K_{5,3}$

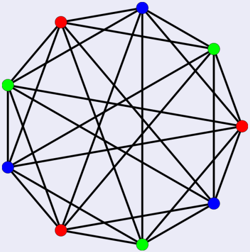


Multipartite graphs

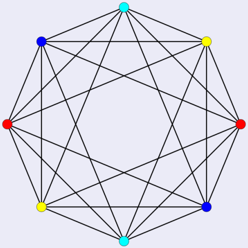
In the complete multipartite graph $K_{n_1,n_2,\ldots,n_r}$, the vertices are coloured in r colours with n_i vertices of colour i and each pair of vertices of different colour is adjacent.



$K_{2,2,2}$



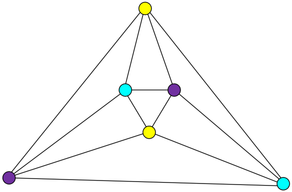
$K_{3,3,3}$



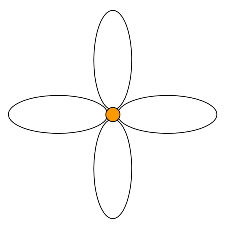
$K_{2,2,2,2}$

Quick quiz

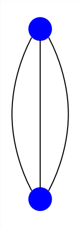
Do you recognise this graph?



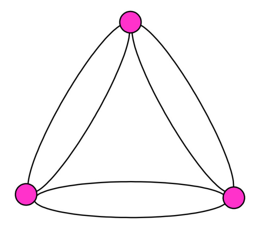
Some standard types of multigraphs



B_4



${K_2}^{\{3\}}$



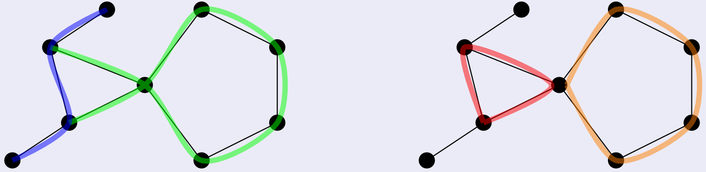
${K_3}^{\{2\}}$

- The bouquet B_n has n loops at a single vertex.
- The complete multigraph ${K_n}^{\{m\}}$ has n vertices and each pair of vertices is connected by m edges.

Traversing a graph

Walks, paths and cycles

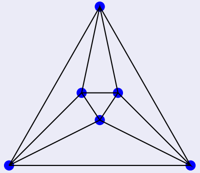
- A walk from X to Y is an alternating sequence $X = X_0, e_1, X_1, e_2, \ldots, X_{l-1}, e_l, X_l = Y$ such that e_i is an edge with endpoints X_{i-1} and X_i.



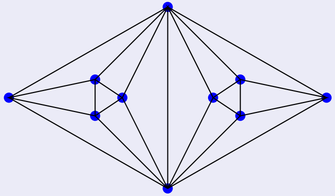
- In a closed walk, the initial and terminal vertex coincide.
- A path is a walk in which each vertex occurs only once, except that the initial and terminal vertex are allowed to coincide.
- A cycle is a closed path.
- The number l of edges is called the length of the walk.
- The distance between two vertices X, Y is the length of the shortest path between them and is denoted by $d(X, Y)$.

Vertex-connectivity

- A graph is called connected if any pair of vertices is connected by a walk (actually by a path, why?).
- A graph is called k-connected if it remains connected whenever fewer than k vertices (and their incident edges) are removed. The 1-connected graphs are precisely the connected graphs.
- The largest k such that $\mathcal{G}$ is k-connected is called the connectivity $\kappa(\mathcal{G})$ of $\mathcal{G}$.



$\kappa(\mathcal{G}) = 4$

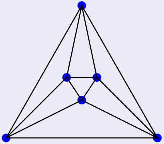


$\kappa(\mathcal{G}) = 2$

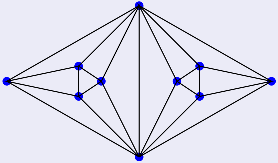
- Equivalent definition: A graph is k-connected if there exist at least k independent paths between every pair of vertices. (Two paths between X and Y are called independent if they only share the initial and terminal vertex.)

Edge-connectivity

- A graph is called l-edge-connected if it remains connected whenever fewer than l edges (but not their incident vertices) are removed.
- The largest l such that $\mathcal{G}$ is l-edge-connected is called the edge-connectivity $\lambda(\mathcal{G})$ of $\mathcal{G}$.
- **Lemma:** $\kappa(\mathcal{G}) \leq \lambda(\mathcal{G}) \leq \delta(\mathcal{G})$, where $\delta(\mathcal{G})$ is the minimal degree of a vertex of $\mathcal{G}$.



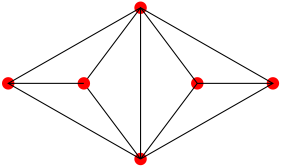
$\kappa(\mathcal{G}) = 4$
$\lambda(\mathcal{G}) = 4$



$\kappa(\mathcal{G}) = 2$
$\lambda(\mathcal{G}) = 4$

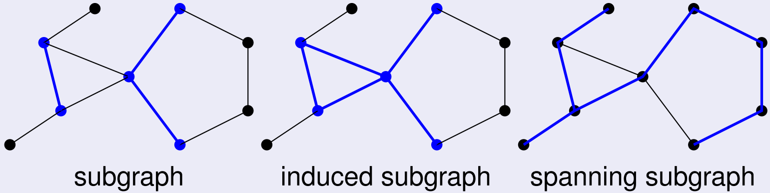
Quick quiz

Determine $\kappa(\mathcal{G})$ and $\lambda(\mathcal{G})$ for this graph.



Subgraphs

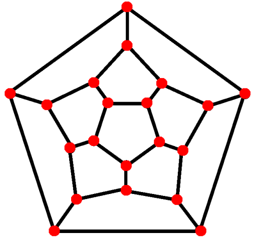
- A subgraph $\mathcal{H}$ of a graph $\mathcal{G}$ has $\mathcal{V}(\mathcal{H}) \subseteq \mathcal{V}(\mathcal{G})$ and $\mathcal{E}(\mathcal{H}) \subseteq \mathcal{E}(\mathcal{G})$ such that the endpoints of each $e \in \mathcal{E}(\mathcal{H})$ lie in $\mathcal{V}(\mathcal{H})$.

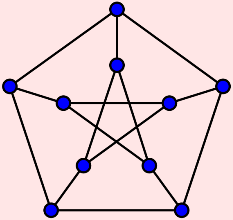


- A subgraph $\mathcal{H}$ is called an induced subgraph if $\mathcal{E}(\mathcal{H})$ contains all edges of $\mathcal{G}$ having both endpoints in $\mathcal{V}(\mathcal{H})$.
- The maximal connected induced subgraphs of a graph are called its (connected) components.
- A subgraph $\mathcal{H}$ of $\mathcal{G}$ containing all vertices of $\mathcal{G}$ is called a spanning (sub)graph of $\mathcal{G}$.

Exercise: Hamiltonian circuits

A graph with a spanning cycle is called a Hamiltonian graph, the spanning cycle is called a Hamiltonian circuit. A Hamiltonian circuit is thus a closed walk that visits every vertex precisely once.

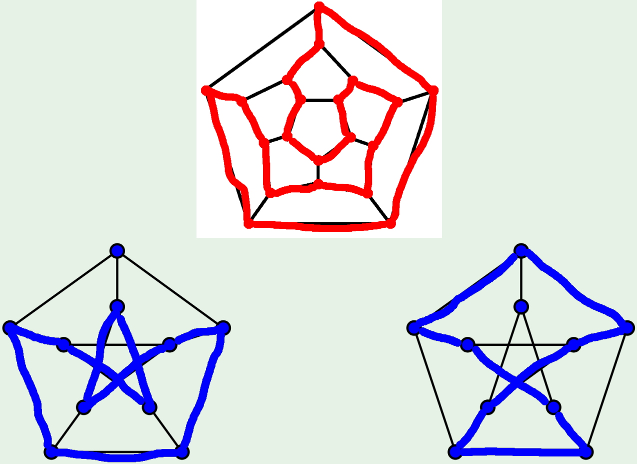




- Find a Hamiltonian circuit in the dodecahedral graph (left).
- The Petersen graph (right) has no Hamiltonian circuit (proving this is somewhat tedious).
  However, if one of the vertices (and its incident edges) is removed, the resulting graph has a Hamiltonian circuit.

  Demonstrate this for one of the interior and for one of the exterior vertices removed.

Solution: Hamiltonian circuits

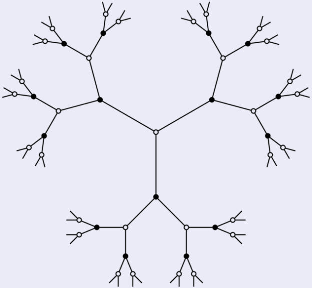


Acyclic graphs

Definition

A graph without cycles is called a forest, a connected graph without cycles is called a tree.

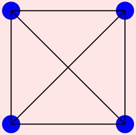
Some important properties of trees



- A tree with n vertices has $n-1$ edges.
- Any two vertices in a tree are connected by a unique path.
- Removing any edge from a tree disconnects it.
- Adding an edge between two vertices of a tree creates a cycle.
- Every tree is a bipartite graph.
- Every connected graph contains a spanning tree (omit edges from cycles until there are no cycles left).

Exercise: Small trees

- How many spanning trees does the complete graph K_4 contain?

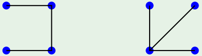


- How many of these are essentially different (i.e. have different adjacency relations)?
- A tree with $n + 1$ vertices can be obtained from a tree with n vertices by adding a new vertex with a new edge to one of the vertices (i.e. by growing a new vertex).

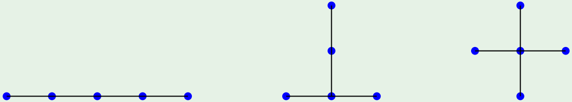
  Use this (and the fact that a tree with 3 vertices is necessarily a linear graph) to enumerate all essentially different trees with 4, 5 and 6 vertices.

Solution: Small trees

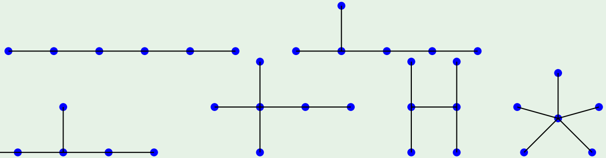
- A spanning tree has 3 edges, there are $\binom{6}{3} = 20$ ways to select 3 of the 6 edges, but 4 of these choices result in a cycle (triangle), thus there are 16 spanning trees.
  Cayley's formula: K_n has n^{n-2} spanning trees.
- There are only two essentially different spanning trees, one is a linear graph and one has a vertex of degree 3:



- $n = 5$:



- $n = 6$:



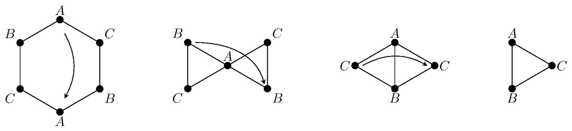
Morphisms of graphs

Definition

A morphism between two graphs $\mathcal{G}$ and $\mathcal{H}$ is a pair of mappings $\phi_{\mathcal{V}} : \mathcal{V}(\mathcal{G}) \to \mathcal{V}(\mathcal{H})$ and $\phi_{\mathcal{E}} : \mathcal{E}(\mathcal{G}) \to \mathcal{E}(\mathcal{H})$ such that the image $\phi_{\mathcal{E}}(e)$ of an edge e with endpoints X, Y has endpoints $\phi_{\mathcal{V}}(X), \phi_{\mathcal{V}}(Y)$.

Morphisms of simple graphs

- For simple graphs, a morphism is fully determined by the mapping $\phi_{\mathcal{V}}$ of the vertices, since $\phi_{\mathcal{V}}(X)$ and $\phi_{\mathcal{V}}(Y)$ are joined by a unique edge (if X and Y are adjacent).
- An elementary morphism of a simple graph identifies two nonadjacent vertices.
  Lemma: Every morphism of a simple graph can be obtained as a sequence of elementary morphisms.

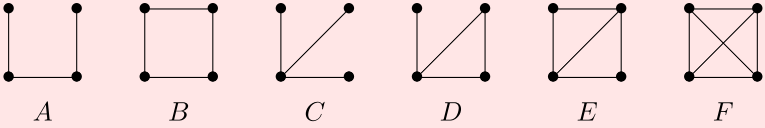


Isomorphisms and automorphisms

- If both mappings $\phi_{\mathcal{V}}$ and $\phi_{\mathcal{E}}$ of a morphism are bijective, the morphism is called an isomorphism and the two graphs $\mathcal{G}$ and $\mathcal{H}$ are called isomorphic. Notation: $\mathcal{G} \cong \mathcal{H}$.
- An isomorphism of a graph $\mathcal{G}$ to itself is called an automorphism. The full group of automorphisms of $\mathcal{G}$ is denoted by $Aut(\mathcal{G})$.
- The automorphisms of a simple graph are the permutations of the vertices which are compatible with the adjacency relation.

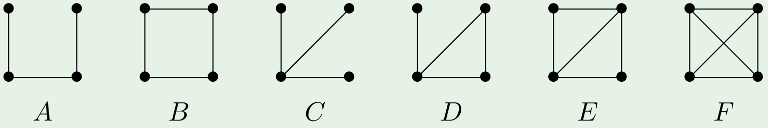
Exercise: Small automorphism groups

Determine the automorphism groups of the six connected simple graphs with 4 vertices.



Solution: Small automorphism groups

It is often useful to determine the orbit and the stabiliser of one vertex under the automorphism group.



A: $Aut(\mathcal{G}) \cong \mathbb{Z}_2$, only reflection possible.

B: $Aut(\mathcal{G}) \cong D_4$, all automorphisms are geometric.

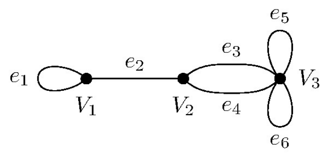
C: $Aut(\mathcal{G}) \cong S_3$, all permutations of degree 1 vertices.

D: $Aut(\mathcal{G}) \cong \mathbb{Z}_2$, only swapping of degree 2 vertices.

E: $Aut(\mathcal{G}) \cong \mathbb{Z}_2 \times \mathbb{Z}_2$, all automorphisms are geometric.

F: $Aut(\mathcal{G}) \cong S_4$, all permutations are allowed.

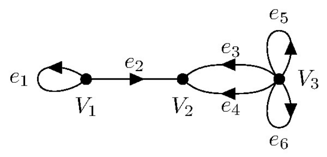
Automorphisms for general graphs



In this graph, $\phi_{\mathcal{V}}$ is necessarily trivial, but $\phi_{\mathcal{E}}$ may (independently) swap the edges e_3 and e_4 and the loops e_5 and e_6.

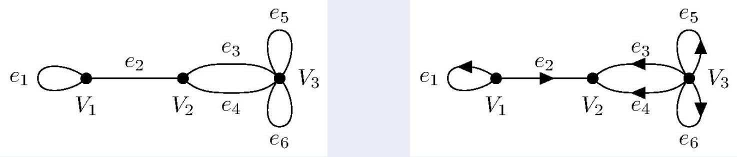
Problem: A loop has two ends, contributing 2 to the degree of a vertex. The reversal of a loop by swapping its ends is not covered by our current definition of a graph automorphism.

A convenient way to introduce this new type of automorphism is to endow the graph with an orientation by assigning a direction to each edge.



Unlike in directed graphs, an oriented edge can still be traversed in both directions.

Turning an undirected graph into an oriented graph



- An orientation assigns a direction to each edge of a graph by considering it as an ordered pair (X, Y) directed from X to Y.
- A directed edge (X, Y) is called an arc, its initial vertex X is called its tail (or source), its terminal vertex Y its head (or target). Correspondingly, arcs are usually represented by arrows.
- A graph $\mathcal{G}$ with edge set $\mathcal{E}(\mathcal{G})$ is turned into an oriented graph by assigning to each edge $e = \{X, Y\}$ an orientation (X, Y):
  - denote the arc (X, Y) with positive orientation by e^+;
  - denote the arc (Y, X) with opposite orientation by e^-.

  The set $\mathcal{E}^\pm = \{e^+, e^- \mid e \in \mathcal{E}(\mathcal{G})\}$ is called the arc set of the oriented graph.
- The mapping $\iota : e^+ \to e^-, e^- \to e^+$ reversing each arc is called the reversal of the orientation.

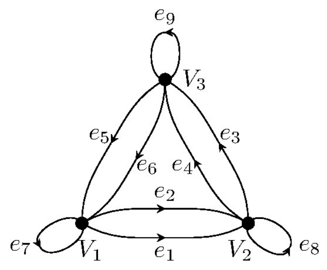
Definition

Let $\mathcal{G}$ be a graph with an orientation resulting in an arc set $\mathcal{E}^{\pm}$.
An automorphism of $\mathcal{G}$ is a pair of bijections $\phi_{\mathcal{V}}$ and $\phi_{\mathcal{E}}$ of $\mathcal{V}(\mathcal{G})$ and $\mathcal{E}^{\pm}$, respectively, such that the image $\phi_{\mathcal{E}}(e)$ of an arc $e = (X, Y)$ is the arc $(\phi_{\mathcal{V}}(X), \phi_{\mathcal{V}}(Y))$.
Moreover, $\phi_{\mathcal{E}}$ must be invariant under reversal of the orientation, i.e. first applying ι and then $\phi_{\mathcal{E}}$ is the same as first applying $\phi_{\mathcal{E}}$ and then ι.
This means: if $(e_{i_1}^{\epsilon_1}, e_{i_2}^{\epsilon_2}, \ldots, e_{i_r}^{\epsilon_r})$ with $\epsilon_i \in \pm$ is a permutation cycle in $\phi_{\mathcal{E}}$, then also $(e_{i_1}^{-\epsilon_1}, e_{i_2}^{-\epsilon_2}, \ldots, e_{i_r}^{-\epsilon_r})$ is a cycle in $\phi_{\mathcal{E}}$.

Some important properties

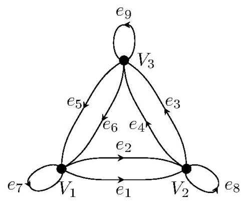
- Every automorphism is fully determined by $\phi_{\mathcal{E}}$.
- The $\phi_{\mathcal{E}}$ fixing all vertices form a normal subgroup K of $Aut(\mathcal{G})$.
- The quotient group $Aut(\mathcal{G})/K$ corresponds to the vertex automorphism group $Aut_{\mathcal{V}}(\mathcal{G})$ induced by the mappings $\phi_{\mathcal{V}}$.
- $Aut_{\mathcal{V}}(\mathcal{G})$ can be identified with a subgroup of $Aut(\mathcal{G})$ having trivial intersection with K, therefore $Aut(\mathcal{G})$ is the semidirect product $K \rtimes Aut_{\mathcal{V}}(\mathcal{G})$ of K by $Aut_{\mathcal{V}}(\mathcal{G})$.

Exercise: Automorphism group



- Determine the vertex automorphism group of the above graph.
- What is the group of automorphisms fixing all vertices, what are generators for this group?
- What is the order of the automorphism group of the graph?
- Give explicitly an automorphism of order 6 of the graph.

Solution: Automorphism group



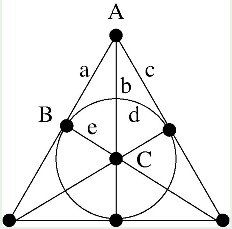
- The vertex automorphism group consists of all $3! = 6$ permutations of the three vertices.
- Generators of the group fixing all vertices are (e_1^+, e_2^+), (e_3^+, e_4^+), (e_5^+, e_6^+) (with the opposite edges mapped accordingly) and (e_7^+, e_7^-), (e_8^+, e_8^-), (e_9^+, e_9^-).
  In total, this is the direct product $\mathbb{Z}_2^6$ of six copies of $\mathbb{Z}_2$.
- The order of the full automorphism group is $2^6 \cdot 3! = 384$.
- An automorphism of order 6 is $(e_1^+, e_3^+, e_5^+)(e_2^+, e_4^+, e_6^+)(e_7^+, e_8^-, e_9^+, e_7^-, e_8^+, e_9^-)$.

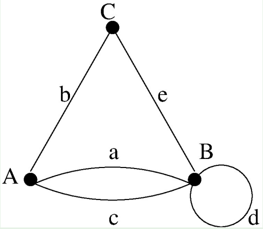
Quotient graphs.

Graph of the orbits

- Let Γ be a subgroup of $Aut(\mathcal{G})$. Denote by $[X]$ the orbit of a vertex X under Γ and by $[e]$ the orbit of an edge e.
- The graph $\mathcal{Q} = \mathcal{Q}(\mathcal{G}, \Gamma) = \mathcal{G}/\Gamma$ having the vertex orbits $[X]$ as its vertices and the edge orbits $[e]$ as its edges is called the quotient graph (with respect to Γ).
  Two vertices $[X], [Y]$ are adjacent in $\mathcal{Q}$ if X', Y' are adjacent in $\mathcal{G}$ for some $X' \in [X]$ and $Y' \in [Y]$.

Example: Rotation of order 3 on the Fano plane graph





Simple quotient graphs

- Vertices at distance 1 (i.e. adjacent) lying in the same orbit give rise to loops in the quotient graph.
- Vertices at distance 2 in the same orbit result in multiple edges in the quotient graph.
- Conclusion: If the quotient graph is required to be a simple graph, vertices in the same orbit need to have at least distance 3.

Free actions

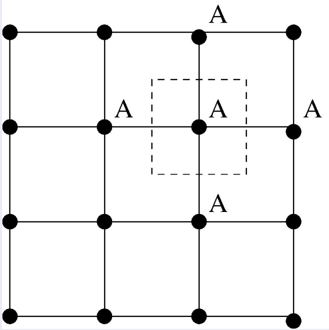
- An automorphism acts freely if it has no fixed points on the vertices and on the edges.
- If all nontrivial automorphism in Γ act freely, then the vertex degrees are preserved in the quotient graph $\mathcal{G}/\Gamma$.
- A typical choice for a subgroup of $Aut(\mathcal{G})$ that acts freely is the group of translations.
  This corresponds to the concept of building up a crystal structure from the unit cell.

The square net

Subgroups acting freely

- Full translation lattice $L = \{m\mathbf{a} + n\mathbf{b} \mid m, n \in \mathbb{Z}\}$.
- Checkerboard sublattice $L' = \{m\mathbf{a} + n\mathbf{b} \in L \mid m + n \text{ even}\}$.
- Scaled sublattices $2L$ and $2L'$.

$L = \{m\mathbf{a} + n\mathbf{b} \mid m, n \in \mathbb{Z}\}$.



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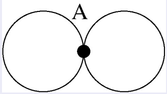
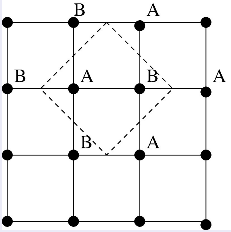


$\mathcal{Q} \cong B_2$

$\mathrm{Aut}(\mathcal{Q}) = \mathbb{Z}_2^2 \rtimes \mathbb{Z}_2$

$|\,\mathrm{Aut}(\mathcal{Q})| = 8$

$L' = \{m\mathbf{a} + n\mathbf{b} \mid m, n \in \mathbb{Z}, m + n \in 2\mathbb{Z}\}$.



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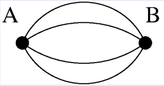
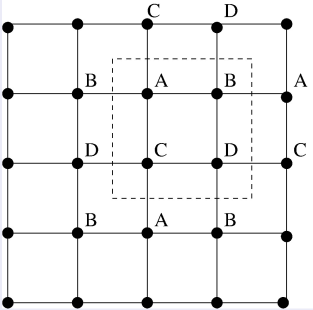


$\mathcal{Q} \cong K_2^{\{4\}}$

$\mathrm{Aut}(\mathcal{Q}) = S_4 \rtimes \mathbb{Z}_2$

$|\,\mathrm{Aut}(\mathcal{Q})| = 48$

$2L = \{m\mathbf{a} + n\mathbf{b} \mid m, n \in 2\mathbb{Z}\}$.



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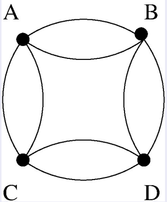
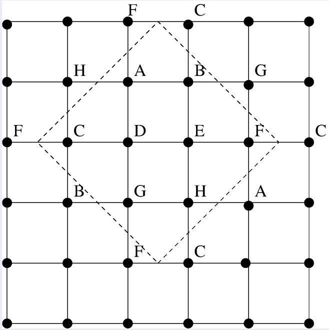


$\mathcal{Q} \cong C_4^{\{2\}}$

$\mathrm{Aut}(\mathcal{Q}) = \mathbb{Z}_2^4 \rtimes D_4$

$|\,\mathrm{Aut}(\mathcal{Q})| = 128$

$2L' = \{m\mathbf{a} + n\mathbf{b} \mid m, n \in 2\mathbb{Z}, m + n \in 4\mathbb{Z}\}$.



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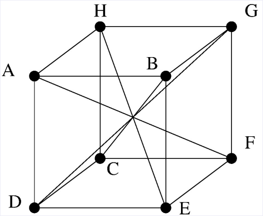
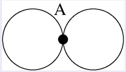
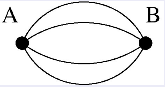


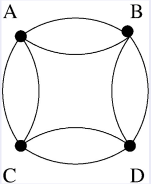
$\mathcal{Q} \cong K_{4,4}$

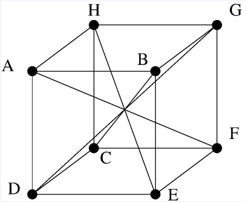
$|\operatorname{Aut}(\mathcal{Q})| = 1152$

Summary: Series of quotients for the square net

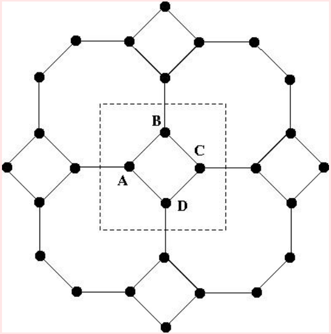


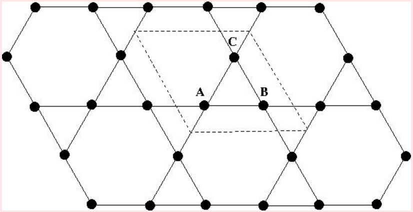






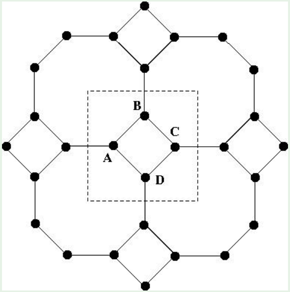
Exercise: Quotient graphs





- Determine the quotient graphs of the Archimedean nets of type 4.8^2 (left) and $3.6.3.6$ (right) with respect to the translation subgroup indicated by the unit cell.
- Also, determine the automorphism groups of the quotient graphs.

Solution: Quotient graphs



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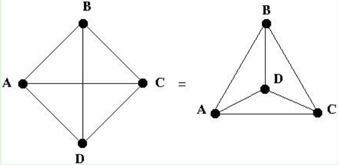
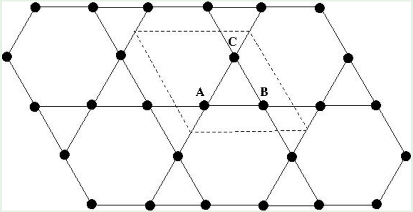


$\mathcal{Q} \cong K_4$

$\mathrm{Aut}(\mathcal{Q}) = S_4$

$|\,\mathrm{Aut}(\mathcal{Q})| = 24$



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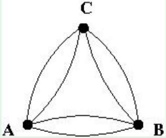


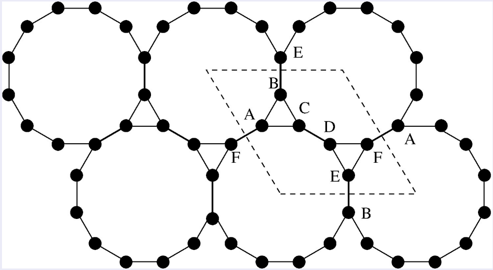
$\mathcal{Q} \cong K_3^{\{2\}}$

$\mathrm{Aut}(\mathcal{Q}) = \mathbb{Z}_2^3 \rtimes D_3$

$|\,\mathrm{Aut}(\mathcal{Q})| = 48$

Non-translational automorphisms acting freely

Archimedean net 3.12^2



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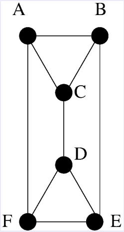
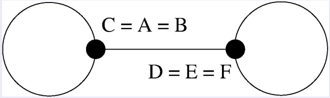
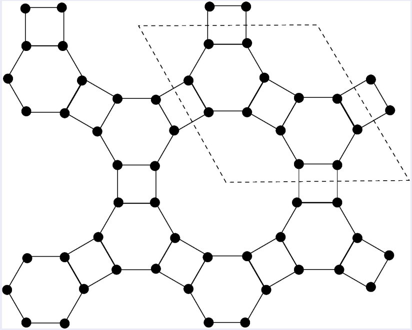


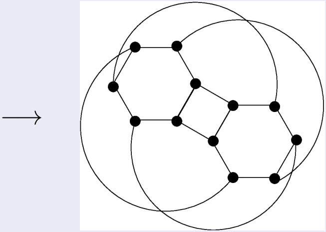
Fixed-point free rotation of order 3

center of rotation: center of dodecagon or center of triangle



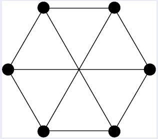
Archimedean net $4.6.12$



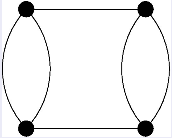


Fixed-point free rotations (around center of dodecagon)

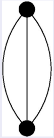
order 2



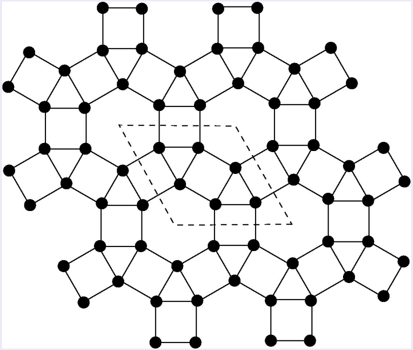
order 3



order 6



Archimedean net $3.4.6.4$



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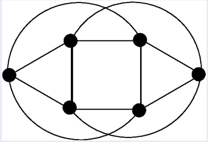
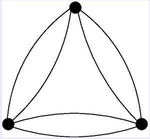
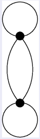


Fixed-point free rotations (around center of hexagon)

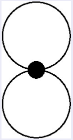
order 2



order 3



order 6

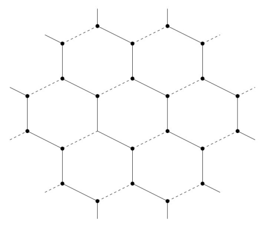


Periodic nets

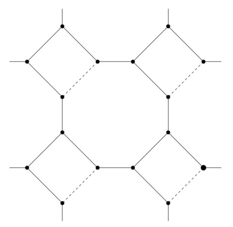
Definition

- A net $\mathcal{N}$ is a simple 3-connected graph, which is locally finite (i.e. every vertex has finite degree).
- A net $\mathcal{N}$ is called p-periodic if it has an embedding into $\mathbb{R}^n$ (for $n \geq p$) such that $Aut(\mathcal{N})$ contains translations in p independent directions.
- Embedding-independent definition: A p-periodic net is a pair $(\mathcal{N}, T)$ of a net $\mathcal{N}$ and a subgroup $T \leq Aut(\mathcal{N})$ such that $T \cong \mathbb{Z}^p$ (i.e. T is free abelian of rank p) and T has finitely many orbits on both the vertices and the edges of $\mathcal{N}$.
- A p-periodic net is called a minimal net if the deletion of any edge and its translates disconnects it into $(p-1)$-periodic subgraphs.

Minimal vs. non-minimal nets



minimal honeycomb net 6^3



non-minimal net 4.8^2

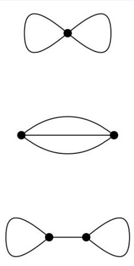
The cyclomatic number

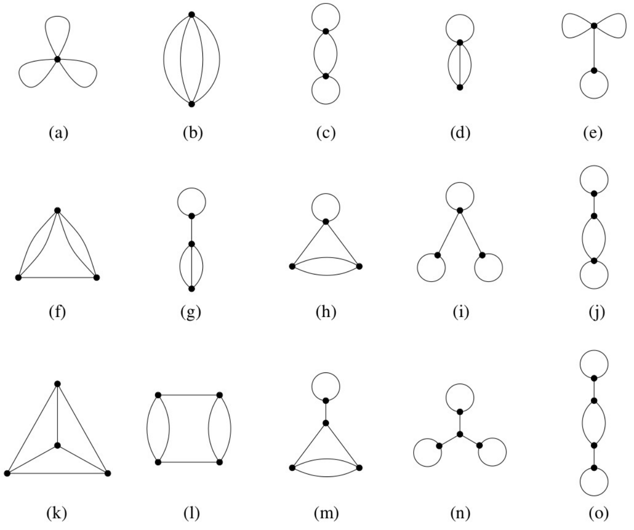
In a connected graph of order n and size m, a spanning tree has $n - 1$ edges and adding p further edges creates p independent cycles. The number $p = m - (n - 1)$ is called the cyclomatic number of the graph.

Consequence

The quotient graph of a minimal p-periodic net of order n has $n - 1 + p$ edges, hence there are only finitely many minimal p-periodic nets.

Quotient graphs of the 2- and 3-dimensional minimal nets



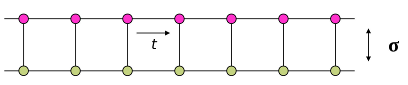


Note: B_2 belongs to the square net and ${K_2}^{\{3\}}$ to the honeycomb net, but the dumbbell graph does not belong to a planar net.

Crystallographic nets

- An n-dimensional crystallographic space group Γ is a group with a normal subgroup $T \cong \mathbb{Z}^n$ such that Γ/T is finite and T coincides with its centraliser in Γ (i.e. T is maximal abelian).
- A crystallographic net is a net whose automorphism group is isomorphic to a crystallographic space group.
- Alternative characterisation:
  - A local automorphism of a net $\mathcal{N}$ is an automorphism ϕ with a global bound b on the distance $d(X, \phi(X))$ between a vertex and its image.
  - The local automorphisms form a normal subgroup $\Lambda(\mathcal{N})$ of $Aut(\mathcal{N})$.
  - A net $\mathcal{N}$ is a crystallographic net if and only if $\Lambda(\mathcal{N})$ is free abelian (i.e. $\cong \mathbb{Z}^n$ for some n) and has only finitely many orbits on both the vertices and the edges of $\mathcal{N}$.

A non-crystallographic net

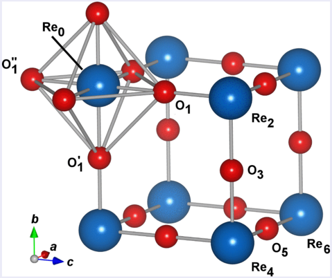


Reflection σ commutes with the translation, but $\langle t, \sigma \rangle \cong \mathbb{Z} \times \mathbb{Z}_2$ is not free abelian.

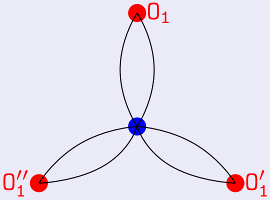
Automorphisms of crystallographic nets

- For a crystallographic net $\mathcal{N}$, the point group $Aut(\mathcal{N})/T$ is isomorphic to a subgroup of the automorphism group $Aut(\mathcal{N}/T)$ of the quotient graph $\mathcal{Q} = \mathcal{N}/T$.
- For a minimal net, $Aut(\mathcal{N})/T$ is isomorphic to $Aut(\mathcal{N}/T)$.
- In the general case, only those automorphisms of $Aut(\mathcal{N}/T)$ are admissible which preserve cycles in $\mathcal{N}$.
  We will come back to this later in the context of voltage graphs.

Example: Rhenium trioxide ($\mathtt{ReO_3}$)

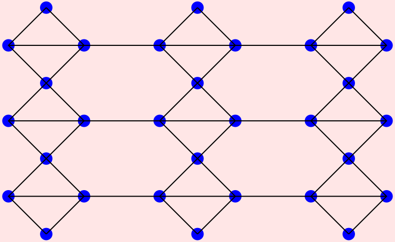


- Translation subgroup T: primitive cubic lattice



- quotient graph $\mathcal{Q} = \mathcal{N}/T \cong {K_{1,3}}^{\{2\}}$
- 1 orbit on $\mathtt{Re}$-atoms
- 3 orbits on $\mathtt{O}$-atoms
- 6 orbits on edges
- point group $Aut(\mathcal{N})/T \cong m\bar{3}m$ is isomorphic to $Aut(\mathcal{Q}) \cong \mathbb{Z}_2^3 \rtimes S_3$

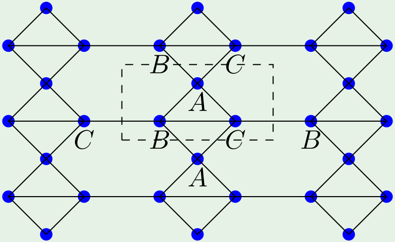
Exercise: The $\beta - W$ net



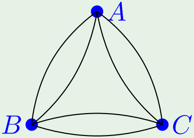
For the $\beta - W$ net $\mathcal{N}$ above, determine

- the translation subgroup T;
- the orbits of T on the vertices and edges;
- the quotient graph $\mathcal{Q} = \mathcal{N}/T$ and its automorphism group;
- the point group $Aut(\mathcal{N})/T$.

Solution: The $\beta - W$ net

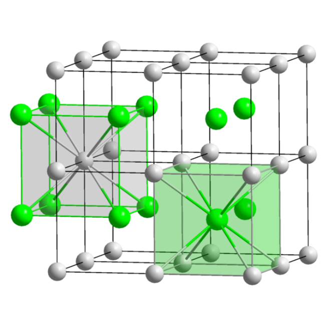


- quotient graph $\mathcal{Q} = \mathcal{N}/T \cong {K_3}^{\{2\}}$
- 1 orbit on A-, B- and C-atoms, respectively
- 6 orbits on edges

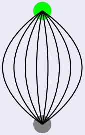


- point group $Aut(\mathcal{N})/T \cong mm2$ (generated by swapping B, C and by swapping the two edges between A and B and between A and C) is isomorphic to a subgroup of $Aut(\mathcal{Q}) \cong \mathbb{Z}_2^3 \rtimes S_3$

Example: Caesium chloride (CsCl)

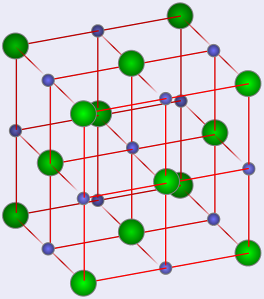


- Translation subgroup T: primitive cubic lattice

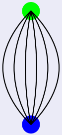


  - quotient graph $\mathcal{Q} = \mathcal{N}/T \cong {K_2}^{\{8\}}$
  - 1 orbit on Cs-atoms
  - 1 orbit on Cl-atoms
  - 8 orbits on edges
- point group $Aut(\mathcal{N})/T \cong m\bar{3}m$ is isomorphic to a subgroup of $Aut(\mathcal{Q}) \cong S_8 \rtimes \mathbb{Z}_2$

Example: Sodium chloride (NaCl)

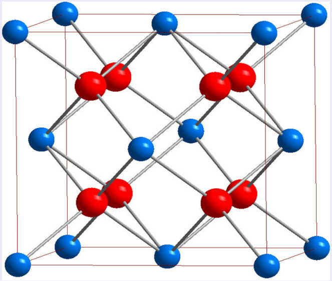


- Translation subgroup T: face centred cubic lattice

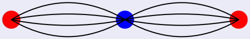


  - quotient graph $\mathcal{Q} = \mathcal{N}/T \cong K_2{}^{\{6\}}$
  - 1 orbit on Na-atoms
  - 1 orbit on Cl-atoms
  - 6 orbits on edges
- point group $Aut(\mathcal{N})/T \cong m\bar{3}m$ is isomorphic to a subgroup of $Aut(\mathcal{Q}) \cong S_6 \rtimes \mathbb{Z}_2$

Example: Calcium fluoride (CaF_2)

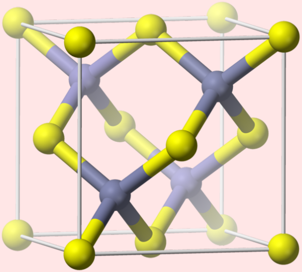


- Translation subgroup T: face centred cubic lattice



  - quotient graph $\mathcal{Q} = \mathcal{N}/T \cong {K_{1,2}}^{\{4\}}$
  - 1 orbit on Ca-atoms
  - 2 orbits on F-atoms
  - 8 orbits on edges
- point group $Aut(\mathcal{N})/T \cong m\bar{3}m$ is isomorphic to a subgroup of $Aut(\mathcal{Q}) \cong S_4^2 \rtimes \mathbb{Z}_2$

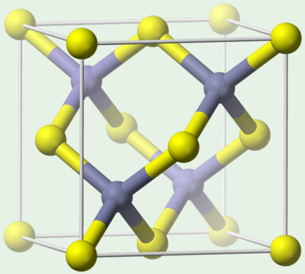
Exercise: Sphalerite (`ZnS`)



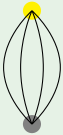
Determine

- the type of the translation subgroup T;
- the orbits on the vertices and edges;
- the quotient graph $\mathcal{Q} = \mathcal{N}/T$ and its automorphism group;
- the point group $Aut(\mathcal{N})/T$.

Solution: Sphalerite (ZnS)



- Translation subgroup T: face centred cubic lattice
- quotient graph $\mathcal{Q} = \mathcal{N}/T \cong K_2{}^{\{4\}}$
- 1 orbit on Zn-atoms
- 1 orbit on S-atoms
- 4 orbits on edges

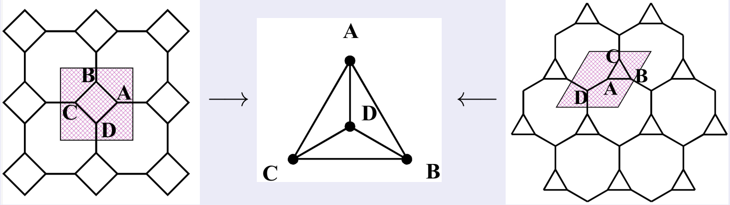


- point group $Aut(\mathcal{N})/T \cong \bar{4}3m$ is isomorphic to the subgroup of $Aut(\mathcal{Q}) \cong S_4 \rtimes \mathbb{Z}_2$ fixing the vertices (which represent different types of atoms)

Two problems and a solution

Two problems

1) Different nets give rise to the same quotient graph.



How can we provide additional information in the quotient graph that distinguishes the different nets?

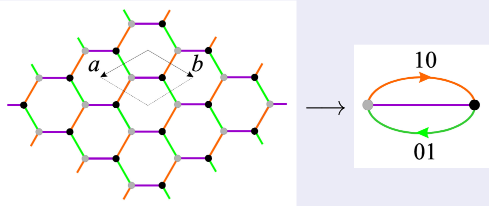
2) How can we reconstruct one or more periodic nets from a given quotient graph?

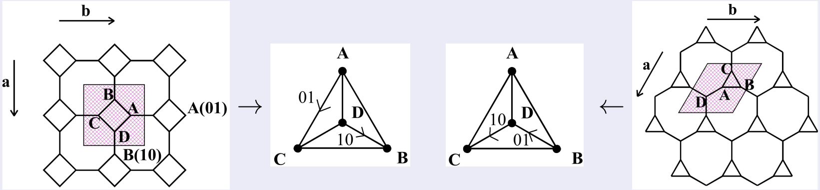
Solution: Voltage graphs

Assign labels to the edges of the quotient graph that correspond to translations in (an embedding of) the underlying net.

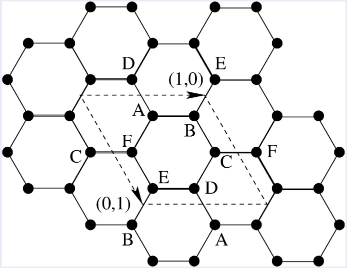
Assigning labels in a voltage graph

- Label the arc (X, Y) in the quotient graph by the translation $\mathbf{t}$ such that $(X, Y + \mathbf{t})$ is an edge in the original periodic net.
- Labels for zero translations (i.e. edges within the unit cell) are omitted.





Voltage graph for the hexagonal net



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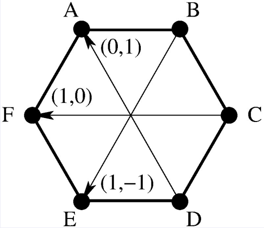
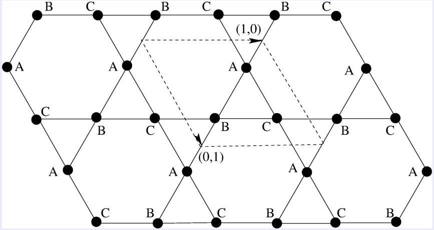


Voltage graph for the Archimedean net $3.6.3.6$



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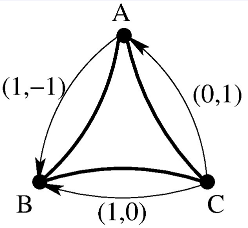
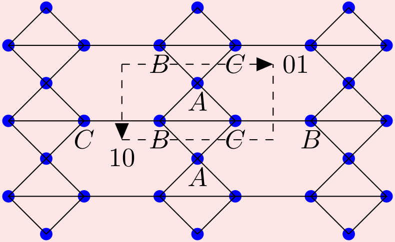
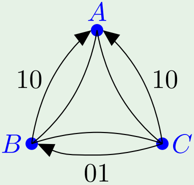


Exercise: Voltage graph for the $\beta - W$ net



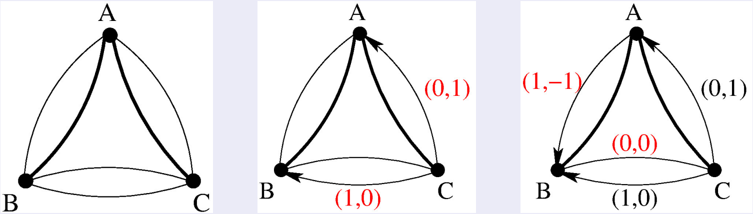
Determine the voltage graph for the $\beta - W$ net with respect to the indicated basis.

Solution: Voltage graph for the $\beta - W$ net



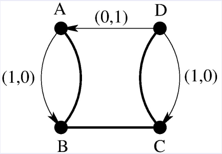
Generating a net from a voltage graph

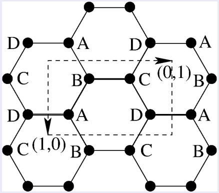
- Choose a spanning tree in the quotient graph and label its edges by zero voltages. This serves as the connected part of the net inside the unit cell.

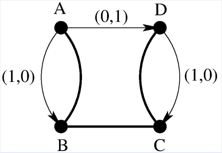


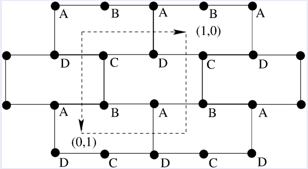
- In order to generate an n-dimensional net, label n edges (not in the spanning tree) by linearly independent translation vectors.
- Choose arbitrary translation vectors (possibly $\mathbf{0}$) for the remaining edges.
- Rules ensuring the generation of a simple graph:
  - Loops at the same vertex must have different labels $\neq \mathbf{0}$.
  - Parallel edges between two vertices must have different labels, anti-parallel edges must not have opposite labels.

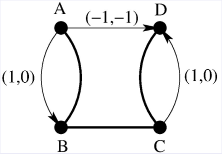
Variations of the hexagonal net

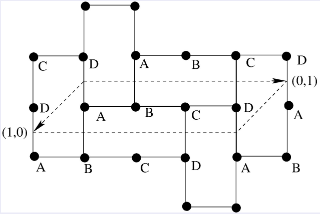










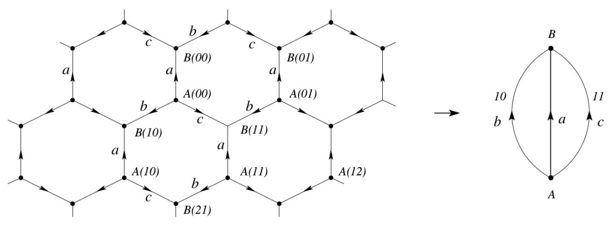


Voltage graphs for minimal nets

- For minimal nets, the assignment of the voltages can be omitted, since the $p = m - (n-1)$ edges not contained in the spanning tree must be assigned p linearly independent translation vectors, i.e. a basis of $\mathbb{R}^p$.
- Different labelling of the edges corresponds to different choices of the unit cell and relabelling of the vertices.
- Recall that for minimal nets $Aut(\mathcal{N})/T$ is isomorphic to $Aut(\mathcal{N}/T)$.

Automorphism groups reloaded

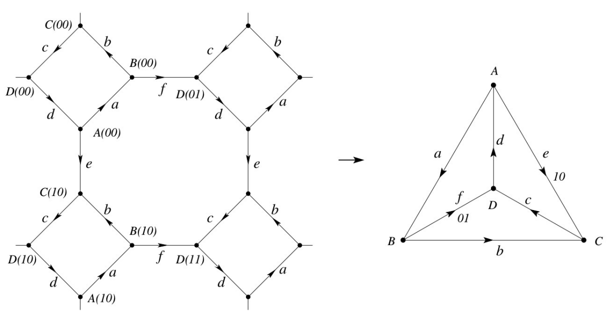
Automorphisms for the honeycomb net 6^3



$Aut(\mathcal{N}/T)$ is generated by
$\sigma_1 = (a^+, b^+, c^+)(a^-, b^-, c^-)$
$\sigma_2 = (a^+, b^+)(a^-, b^-)$
$\sigma_3 = (a^+, a^-)(b^+, b^-)(c^+, c^-)$

Cycle with zero voltage is $w = a^+c^-b^+a^-c^+b^-$:
$\sigma_1(w) = b^+a^-c^+b^-a^+c^- = w$, $\quad \sigma_2(w) = b^+c^-a^+b^-c^+a^- = w^-$,
$\sigma_3(w) = a^-c^+b^-a^+c^-b^+ = w$
$\Rightarrow$ all automorphisms in $Aut(\mathcal{N}/T)$ give rise to automorphisms in $Aut(\mathcal{N})/T$.

Automorphism for the Archimedean net 4.8^2



$Aut(\mathcal{N}/T)$ is generated by

$\sigma_1 = (a^+, b^+, c^+, d^+)(a^-, b^-, c^-, d^-)$ [induced by (A, B, C, D)]

$\sigma_2 = (a^+, d^-)(a^-, d^+)(b^+, c^-)(b^-, c^+)(f^+, f^-)$ [induced by (B, D)]

$\sigma_3 = (a^+, a^-)(b^+, e^+)(b^-, e^-)(d^+, f^-)(d^-, f^+)$ [induced by (A, B)]

Cycle with zero voltage is $w = a^+b^+c^+d^+$:

$\sigma_1(w) = b^+c^+d^+a^+ = w, \quad \sigma_2(w) = d^-c^-b^-a^- = w^-$,

$\sigma_3(w) = a^-e^+c^+f^-$ with voltage $(1, -1)$

$\Rightarrow Aut(\mathcal{N})/T \cong \langle \sigma_1, \sigma_2 \rangle \leq Aut(\mathcal{N}/T)$

Cycle and cocycle spaces

- For a finite graph $\mathcal{G}$ with edges $\mathcal{E} = \{e_1, \ldots, e_m\}$, the $\mathbb{Z}$-linear combinations $\sum_{i=1}^{m} \lambda_i e_i$ with $\lambda_i \in \mathbb{Z}$ form a $\mathbb{Z}$-module $\mathfrak{L}_{\mathcal{E}}$, called the 1-chain space.
- The 1-chains corresponding to cycles in $\mathcal{G}$ are called cycle vectors and span the cycle space $\mathfrak{C} = \mathfrak{C}(\mathcal{G}) \subseteq \mathfrak{L}_{\mathcal{E}}$.
- The coboundary operator δ assigns to a vertex $X \in \mathcal{V}(\mathcal{G})$ the star vector

  $$\delta(X) = \sum_{e \in \mathcal{E}} \epsilon_e e \quad \text{with} \quad \epsilon_e = \begin{cases} 1 & \text{if } X \text{ is the tail of } e; \\ -1 & \text{if } X \text{ is the head of } e; \\ 0 & \text{if } X \text{ is not incident with } e. \end{cases}$$

  Thus, $\delta(X)$ is the sum of arcs incident with X, taken positive for outgoing and negative for incoming arcs.
- The subspace of $\mathfrak{L}_{\mathcal{E}}$ spanned by the $\delta(X)$ is called the cocycle space or cut space and is denoted by $\mathfrak{C}^* = \mathfrak{C}^*(\mathcal{G})$.

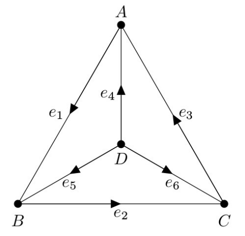
Properties of the cycle and cocycle spaces $\mathfrak{C}$ and $\mathfrak{C}^*$

- Considering the edges e_i as an orthonormal basis of $\mathfrak{L}_{\mathcal{E}}$, i.e. $e_i \cdot e_j = \delta_{ij}$, $\mathfrak{C}$ and $\mathfrak{C}^*$ are orthogonal complements of each other:

$$\mathfrak{L}_{\mathcal{E}} = \mathfrak{C} \oplus \mathfrak{C}^*, \quad \mathfrak{C}^{\perp} = \mathfrak{C}^*, \quad (\mathfrak{C}^*)^{\perp} = \mathfrak{C}.$$

- $\sum_{X \in \mathcal{V}} \delta(X) = 0$, since every edge occurs once in both orientations.
- $\dim \mathfrak{C}^* = n - 1$ and a basis of $\mathfrak{C}^*$ are the star vectors $\delta(X)$ running over all but one vertex.
- $\dim \mathfrak{C} = m - n + 1$ is equal to the cyclomatic number of $\mathcal{G}$.
- For a partition $\mathcal{V} = \mathcal{V}_1 \cup \mathcal{V}_2$ of the vertices, the arcs with tail in $\mathcal{V}_1$ and head in $\mathcal{V}_2$ are called a cut and the corresponding sum in $\mathfrak{L}_{\mathcal{E}}$ is called a cut vector.
  The special partitions $\mathcal{V}_1 = \{X\}$ and $\mathcal{V}_2 = \mathcal{V} \setminus \{X\}$ give the star vector $\delta(X)$.
- All cut vectors are linear combinations of the star vectors.

Example: K_4



$n = 4$ vertices, $m = 6$ edges $\Rightarrow \dim \mathfrak{C} = 3$

basis of $\mathfrak{C}$

$e_1 + e_4 - e_5$

$e_2 + e_5 - e_6$

$e_3 - e_4 + e_6$

basis of $\mathfrak{C}^*$

$\delta(A) = e_1 - e_3 - e_4$

$\delta(B) = -e_1 + e_2 - e_5$

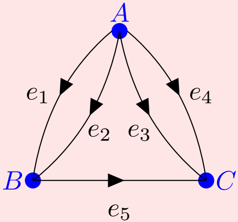
$\delta(C) = -e_2 + e_3 - e_6$

Cycle-cocycle basis

$$M = \begin{pmatrix} 1 & 0 & 0 & 1 & -1 & 0 \\ 0 & 1 & 0 & 0 & 1 & -1 \\ 0 & 0 & 1 & -1 & 0 & 1 \\ 1 & 0 & -1 & -1 & 0 & 0 \\ -1 & 1 & 0 & 0 & -1 & 0 \\ 0 & -1 & 1 & 0 & 0 & -1 \end{pmatrix}$$

basis transformation matrix M: rows express the combined bases for $\mathfrak{C}$ and $\mathfrak{C}^*$ in terms of the standard basis of $\mathfrak{L}_{\mathcal{E}}$.

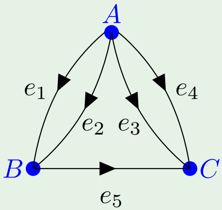
Exercise: Cycle and cocycle space



For the graph given above, determine:

- the dimensions of the cycle space $\mathfrak{C}$ and the cocycle space $\mathfrak{C}^*$;
- a basis for the cycle space $\mathfrak{C}$;
- a basis for the cocycle space $\mathfrak{C}^*$;
- the matrix M containing as rows the combined bases for $\mathfrak{C}$ and $\mathfrak{C}^*$ in terms of the standard basis of $\mathfrak{L}_{\mathcal{E}}$.

Solution: Cycle and cocycle space



- $n = 3$, $m = 5 = \dim \mathfrak{L}_{\mathcal{E}}$
  $\Rightarrow \dim \mathfrak{C} = m - (n-1) = 3,\ \dim \mathfrak{C}^* = n - 1 = 2$
- three independent cycles are: $e_1 - e_2, \quad e_3 - e_4, \quad e_2 + e_5 - e_3$
- star vectors: $\delta(A) = e_1 + e_2 + e_3 + e_4, \quad \delta(B) = -e_1 - e_2 + e_5$
- $M = \begin{pmatrix} 1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 \\ 0 & 1 & -1 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 \\ -1 & -1 & 0 & 0 & 1 \end{pmatrix}$

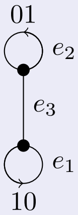
Specifying an embedding from a voltage graph

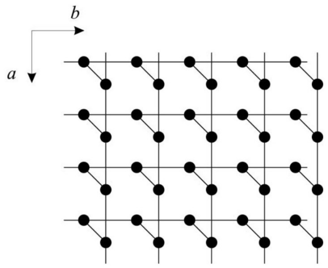
- The voltages are vectors in $\mathbb{R}^p$.
- An embedding α into $\mathbb{R}^r$ with $r \geq p$
  - assigns to each vertex X a point $\alpha(X) \in \mathbb{R}^r$,
  - maps the arc $e = (X, Y)$ to $\alpha(e) = \alpha(Y) - \alpha(X)$,
  - maps a basis of the voltage space $\mathbb{R}^p$ to p linearly independent vectors in $\mathbb{R}^r$.
- Boundary condition: for each cycle w, $\alpha(w)$ must coincide with the image of the voltage of this cycle.
- Thus, the voltages fully determine α on the cycle space $\mathfrak{C}$, the freedom lies in the mapping of the cocycle space $\mathfrak{C}^*$.
- For that, assign to each vertex V_i a vector $L_i^* = \alpha(\delta(V_i)) \in \mathbb{R}^r$ such that $\sum_{i=1}^n L_i^* = 0$ (recall that $\sum_{i=1}^n \delta(V_i) = 0$).
  The set of L_i^* is called a co-lattice in $\mathbb{R}^r$, its span can have any dimension between 0 and $\min(r, n-1)$.
- Consequence: An embedding for a voltage graph is determined by choosing a lattice basis of rank p and a co-lattice in $\mathbb{R}^r$.

Some conventions and terminology on embeddings

- It is convenient (but not necessary) to select a basis of the cycle space having as voltages the standard basis of $\mathbb{R}^p$.
- Often (but not always) one of the vertices is chosen as the origin of the coordinate system.
- An embedding is regarded as a proper embedding if all vertices are mapped to different points in $\mathbb{R}^r$ and if the edges have no crossings.
- An embedding is called a good embedding if the distance between non-adjacent vertices is strictly larger than that between any pair of adjacent vertices.

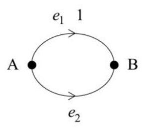
Example of a non-proper embedding





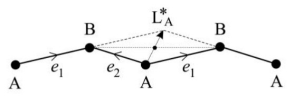
- e_1, e_2 form a basis of the cycle space and e_3 of the cocycle space.
- Any 2-dimensional embedding of this net will have crossings, a barycentric embedding (where each vertex is at the centre of mass of its neighbours) will even not be injective, since the edge e_3 collapses.
- Theorem: A minimal net without a bridge (i.e. a cut consisting of a single edge) has a proper embedding.

Choice of the co-lattice

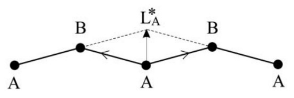


- voltage assignment in $\mathbb{R}^1$, embedding into $\mathbb{R}^2$
- $\mathfrak{C}$ is spanned by $e_1 - e_2$,
  $\mathfrak{C}^*$ is spanned by $\delta(A) = e_1 + e_2$

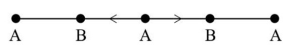
1) arbitrary co-lattice vector L_A^*:
   symmetry of embedding is $\mathfrak{p}211$



2) L_A^* perpendicular to translation $\alpha(e_1 - e_2)$:
   symmetry of embedding is $\mathfrak{p}2mg$



3) $L_A^* = 0$:
   symmetry of embedding is $\mathfrak{p}2mm$
   with translation halved



Barycentric embedding

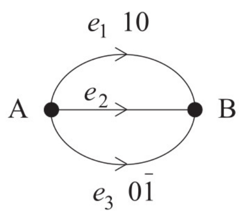
Definition

The special case that all $\delta(V_i)$ and thus all elements of $\mathfrak{C}^*$ are mapped to $\mathbf{0}$ is called the barycentric embedding.

Why is it called the barycentric embedding?

- Since the sum of the outgoing arcs at every vertex is zero, each vertex lies at the centre of mass of its neighbours.
- Conversely, in a non-barycentric embedding, the difference vector $\alpha(V_i) - C$ between an atom and the centre of mass C of its neighbours is equal to $\frac{1}{d_i} L_i^*$ where d_i is the degree of V_i.
- Of the different embeddings, the barycentric embedding has the highest symmetry.

Example: Barycentric embedding of $K_2^{\{3\}}$



basis for $\mathfrak{C}$: $b_1 = e_1 - e_2,$
$b_2 = e_2 - e_3$

basis for $\mathfrak{C}^*$: $b_3 = \delta(A) = e_1 + e_2 + e_3$

cycle-cocycle basis $M = \begin{pmatrix} 1 & -1 & 0 \\ 0 & 1 & -1 \\ 1 & 1 & 1 \end{pmatrix}$

from the voltage graph:

$\alpha(b_1) = \begin{pmatrix} 1 & 0 \end{pmatrix}, \quad \alpha(b_2) = \begin{pmatrix} 0 & 1 \end{pmatrix}, \quad \alpha(b_3) = \mathbf{0}$

Determination of the geometry of the lattice

$$M \cdot M^{\mathsf{T}} = \begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & 0 \\ 0 & 0 & 3 \end{pmatrix}$$

shows that b_1, b_2 form the basis of a hexagonal lattice.

Basis transformation

$$M \cdot \begin{pmatrix} \alpha(e_1) \\ \alpha(e_2) \\ \alpha(e_3) \end{pmatrix} = \begin{pmatrix} \alpha(b_1) \\ \alpha(b_2) \\ \alpha(b_3) \end{pmatrix} \Rightarrow \begin{pmatrix} \alpha(e_1) \\ \alpha(e_2) \\ \alpha(e_3) \end{pmatrix} = M^{-1} \cdot \begin{pmatrix} \alpha(b_1) \\ \alpha(b_2) \\ \alpha(b_3) \end{pmatrix}$$

where $\alpha(b_i)$ can be read off the voltage graph.

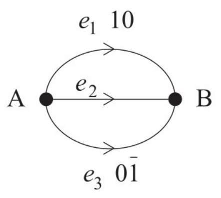
Embedding of the edges

$$M^{-1} = \begin{pmatrix} 1 & -1 & 0 \\ 0 & 1 & -1 \\ 1 & 1 & 1 \end{pmatrix}^{-1} = \frac{1}{3} \begin{pmatrix} 2 & 1 & 1 \\ -1 & 1 & 1 \\ -1 & -2 & 1 \end{pmatrix}$$

$$\begin{pmatrix} \alpha(e_1) \\ \alpha(e_2) \\ \alpha(e_3) \end{pmatrix} = \frac{1}{3} \begin{pmatrix} 2 & 1 & 1 \\ -1 & 1 & 1 \\ -1 & -2 & 1 \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{pmatrix} = \frac{1}{3} \begin{pmatrix} 2 & 1 \\ -1 & 1 \\ -1 & -2 \end{pmatrix}$$

i.e. $\alpha(e_1) = \begin{pmatrix} \frac{2}{3} & \frac{1}{3} \end{pmatrix}$, $\quad \alpha(e_2) = \begin{pmatrix} -\frac{1}{3} & \frac{1}{3} \end{pmatrix}$, $\quad \alpha(e_3) = \begin{pmatrix} -\frac{1}{3} & -\frac{2}{3} \end{pmatrix}$.

Determination of the vertices

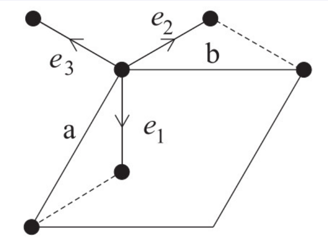


Choosing A at the origin, we obtain

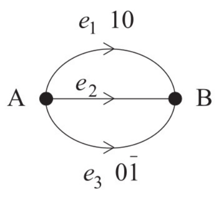
$$\alpha(B) = \alpha(e_2) = \begin{pmatrix} -\frac{1}{3} & \frac{1}{3} \end{pmatrix}$$

and the other two vertices in the orbit of B incident to A are at

$\alpha(e_1) = \begin{pmatrix} \frac{2}{3} & \frac{1}{3} \end{pmatrix}$ and $\alpha(e_3) = \begin{pmatrix} -\frac{1}{3} & -\frac{2}{3} \end{pmatrix}$



Determination of the point and space group type



Automorphisms of the voltage graph induce an action on the cycles and on the corresponding translations:

$\sigma_1 = (e_1, e_2, e_3)$:

$e_1 - e_2 \mapsto e_2 - e_3 \Rightarrow 10 \mapsto 01$

$e_2 - e_3 \mapsto e_3 - e_1 \Rightarrow 01 \mapsto \bar{1}\bar{1}$

$\Rightarrow R(\sigma_1) = \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}$ (3-fold rotation)

$\sigma_2 = (e_1, e_3)$:

$e_1 - e_2 \mapsto e_3 - e_2 \Rightarrow 10 \mapsto 0\bar{1}$

$e_2 - e_3 \mapsto e_2 - e_1 \Rightarrow 01 \mapsto \bar{1}0$

$\Rightarrow R(\sigma_2) = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$

(reflection)

$\sigma_3 = (e_1, -e_1)(e_2, -e_2)(e_3, -e_3)$:

$e_1 - e_2 \mapsto -e_1 + e_2 \Rightarrow 10 \mapsto \bar{1}0$

$e_2 - e_3 \mapsto -e_2 + e_3 \Rightarrow 01 \mapsto 0\bar{1}$

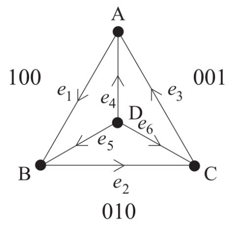
$\Rightarrow R(\sigma_3) = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$

(2-fold rotation)

$\Rightarrow$ point group of type $6mm$.

$\Rightarrow$ space group of type $p6mm$.

Example: Barycentric embedding of K_4



basis for $\mathfrak{C}$: $b_1 = e_1 + e_4 - e_5,$
$b_2 = e_2 + e_5 - e_6,$
$b_3 = e_3 - e_4 + e_6$

basis for $\mathfrak{C}^*$: $b_4 = \delta(A)$, $b_5 = \delta(B)$, $b_6 = \delta(C)$

from the voltage graph: $\alpha(b_1) = \begin{pmatrix}1 & 0 & 0\end{pmatrix}$,
$\alpha(b_2) = \begin{pmatrix}0 & 1 & 0\end{pmatrix}$, $\alpha(b_3) = \begin{pmatrix}0 & 0 & 1\end{pmatrix}$,
$\alpha(b_4) = \alpha(b_5) = \alpha(b_6) = \mathbf{0}$

Determination of the lattice type

$$M \cdot M^{\mathsf{T}} = \begin{pmatrix} 3 & -1 & -1 & 0 & 0 & 0 \\ -1 & 3 & -1 & 0 & 0 & 0 \\ -1 & -1 & 3 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & -1 & -1 \\ 0 & 0 & 0 & -1 & 3 & -1 \\ 0 & 0 & 0 & -1 & -1 & 3 \end{pmatrix}$$

shows that b_1, b_2, b_3 form the basis of a body-centred cubic lattice.

Basis transformation

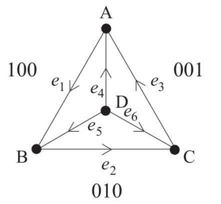
$$M \cdot \begin{pmatrix} \alpha(e_1) \\ \vdots \\ \alpha(e_6) \end{pmatrix} = \begin{pmatrix} \alpha(b_1) \\ \vdots \\ \alpha(b_6) \end{pmatrix} \Rightarrow \begin{pmatrix} \alpha(e_1) \\ \vdots \\ \alpha(e_6) \end{pmatrix} = M^{-1} \cdot \begin{pmatrix} \alpha(b_1) \\ \vdots \\ \alpha(b_6) \end{pmatrix}$$

Embedding of the edges

$$\begin{pmatrix} 1 & 0 & 0 & 1 & -1 & 0 \\ 0 & 1 & 0 & 0 & 1 & -1 \\ 0 & 0 & 1 & -1 & 0 & 1 \\ 1 & 0 & -1 & -1 & 0 & 0 \\ -1 & 1 & 0 & 0 & -1 & 0 \\ 0 & -1 & 1 & 0 & 0 & -1 \end{pmatrix}^{-1} \cdot \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \frac{1}{4} \begin{pmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \\ 1 & 0 & -1 \\ -1 & 1 & 0 \\ 0 & -1 & 1 \end{pmatrix}$$

i.e. $\alpha(e_1) = \begin{pmatrix} \frac{1}{2} & \frac{1}{4} & \frac{1}{4} \end{pmatrix}$, $\alpha(e_2) = \begin{pmatrix} \frac{1}{4} & \frac{1}{2} & \frac{1}{4} \end{pmatrix}, \ldots, \alpha(e_6) = \begin{pmatrix} 0 & -\frac{1}{4} & \frac{1}{4} \end{pmatrix}$
with respect to the primitive basis of the body-centred cubic lattice.

Determination of the vertices



Choosing D at the origin, we obtain

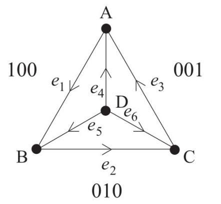
$$\alpha(A) = \alpha(e_4) = \begin{pmatrix}\frac{1}{4} & 0 & -\frac{1}{4}\end{pmatrix}$$
$$\alpha(B) = \alpha(e_5) = \begin{pmatrix}-\frac{1}{4} & \frac{1}{4} & 0\end{pmatrix}$$
$$\alpha(C) = \alpha(e_6) = \begin{pmatrix}0 & -\frac{1}{4} & \frac{1}{4}\end{pmatrix}$$

with respect to the primitive basis of the body-centred cubic lattice.

Transforming this to the primitive cubic basis by the centring matrix

$$W = \frac{1}{2}\begin{pmatrix}-1 & 1 & 1\\ 1 & -1 & 1\\ 1 & 1 & -1\end{pmatrix} \text{ gives } \begin{pmatrix}\alpha(A)\\ \alpha(B)\\ \alpha(C)\end{pmatrix} \cdot W = \begin{pmatrix}-\frac{1}{4} & 0 & \frac{1}{4}\\ \frac{1}{4} & -\frac{1}{4} & 0\\ 0 & \frac{1}{4} & -\frac{1}{4}\end{pmatrix}$$

Determination of the point group type



Automorphisms of K_4 induce an action on the cycles and on the corresponding translations.

$\sigma_1 = (A, B, C, D)$:

$e_1 - e_5 + e_4 \mapsto e_2 + e_3 + e_1 \Rightarrow 100 \mapsto 111$

$e_2 - e_6 + e_5 \mapsto -e_6 + e_4 - e_3 \Rightarrow 010 \mapsto 00\bar{1}$

$e_3 - e_4 + e_6 \mapsto -e_5 - e_1 - e_4 \Rightarrow 001 \mapsto \bar{1}00$

$$\Rightarrow R(\sigma_1) = \begin{pmatrix} 1 & 0 & -1 \\ 1 & 0 & 0 \\ 1 & -1 & 0 \end{pmatrix} \text{ (4-fold rotation)}$$

$$\sigma_2 = (A, B, C) \Rightarrow R(\sigma_2) = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \text{ (3-fold rotation)}$$

$$\sigma_3 = (A, B) \Rightarrow R(\sigma_3) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix} \text{ (2-fold rotation)}$$

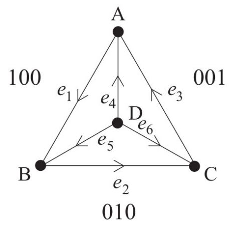
$\Rightarrow$ point group of type 432.

Body-centred cubic lattice $\Rightarrow$ symmetry group of the embedding belongs to the arithmetic class $432I$.

Finding the intrinsic translation part

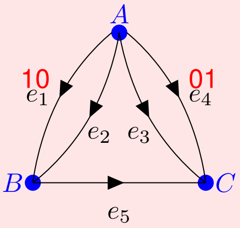
- For a crystallographic symmetry operation $\{R \mid t\}$ with linear part R of order k and translation part t, $\{R \mid t\}^k$ is a pure translation (possibly zero) of the form $\{I \mid t_k\}$ and $\frac{1}{k}t_k$ is called the intrinsic translation part of $\{R \mid t\}$.
- $t_k = t + Rt + R^2t + \ldots + R^{k-1}t$ is the sum over the orbit of t under the cyclic group generated by R.
- Since $\{R \mid t\}$ maps the origin to t, one has to compute the orbit of a walk from the origin to its image:
  let V be the origin and let w be a walk from V to $\sigma(V)$, then $w + \sigma(w) + \ldots + \sigma^{k-1}(w)$ is the cycle corresponding to t_k.

Determination of the space group type



- Choose D as origin and consider $\sigma = \sigma_1 = (A, B, C, D)$, then $\sigma(D) = A$ and e_4 is a walk from D to $\sigma(D)$.
- Orbit of e_4: e_4, e_1, e_2, $-e_6$ $\Rightarrow$ the cycle corresponding to σ^4 is $e_1 + e_2 + e_4 - e_6$.
- This cycle has voltage $110 \Rightarrow \sigma$ is a 4-fold screw rotation with axis along 110.
- Conclusion: space group type is $I4_132$.

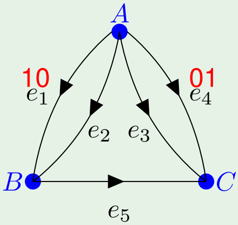
Exercise: Barycentric embedding



For the voltage graph given above, determine a two-dimensional barycentric embedding.

- It is a good idea to put A at the origin.
- To invert a 5×5-matrix, you may use any convenient tool (or ask the lecturer for assistance with a computer algebra system).

Solution: Barycentric embedding

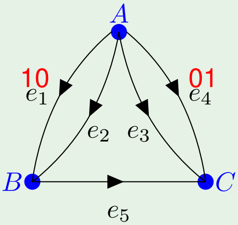


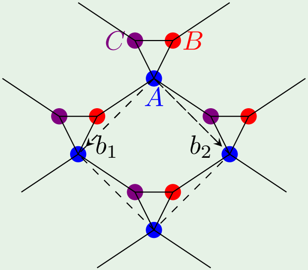
The cycle-cocycle matrix M was already determined in a previous exercise as $M = \begin{pmatrix} 1 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 \\ 0 & 1 & -1 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 \\ -1 & -1 & 0 & 0 & 1 \end{pmatrix}$.

Note that the cycle $b_3 = e_2 - e_3 + e_5$ has zero voltage, hence the embedding of the edges is $M^{-1} \cdot \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} = \frac{1}{8} \begin{pmatrix} 5 & -1 \\ -3 & -1 \\ -1 & -3 \\ -1 & 5 \\ 2 & -2 \end{pmatrix}$.

Solution: Barycentric embedding (ctd.)

Choosing A at the origin, B is at $\alpha(e_2) = \begin{pmatrix} -\frac{3}{8} & -\frac{1}{8} \end{pmatrix}$ and C at $\alpha(e_3) = \begin{pmatrix} -\frac{1}{8} & -\frac{3}{8} \end{pmatrix}$.

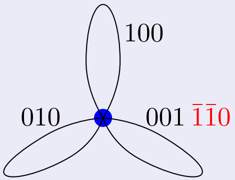




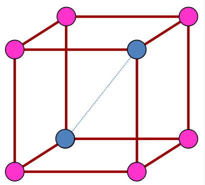
Integral embeddings

- The integral embedding of a minimal net is an embedding into $\mathbb{R}^m$ which assigns the standard basis vectors of $\mathbb{R}^m$ to the edges of the quotient graph of the minimal net.
- Usually, the voltages of an integral embedding are not given explicitly, since different assignments only differ by a permutation of the basis vectors of $\mathbb{R}^m$.
- Since the periodicity of a minimal net is equal to its cyclomatic number $m - n + 1 \leq m$, the integral embedding is usually subperiodic, with finite extension along the cocycle space.
- Integral embeddings can thus be regarded as generalisations of layer structures.
- The main application of integral embeddings is to construct nets as quotients of the minimal net.

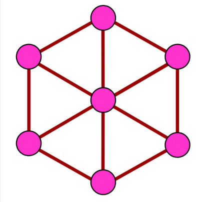
The hexagonal net as a projection of a minimal net



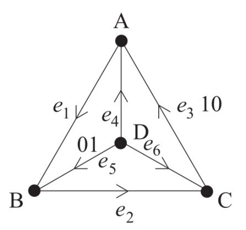
quotient graph of cubic net



- Forming the quotient graph with respect to the subgroup generated by the translation by 111 is equivalent with replacing the voltage 001 by $\bar{1}\bar{1}0$ (and disregarding the third component of the voltages).
- The resulting net is the hexagonal net, obtained as projection of the cubic net along the 111 direction.



Example: Barycentric embedding of 4.8^2 by projection



basis for $\mathfrak{C}$: $$b_1 = e_3 - e_4 + e_6,\quad b_2 = e_2 + e_5 - e_6,\quad b_3 = e_1 + e_2 + e_4 - e_6$$

b_3 has zero voltage $\Rightarrow$ embedding is orthogonal projection along b_3.
Adjust b_1, b_2 such that they are perpendicular to b_3: $b_1' = 2b_1 + b_3$, $b_2' = 2b_2 - b_3$.

basis for $\mathfrak{C}^*$: $$b_4 = \delta(A) = e_1 - e_3 - e_4,\quad b_5 = \delta(B) = -e_1 + e_2 - e_5,\quad b_6 = \delta(C) = -e_2 + e_3 - e_6$$

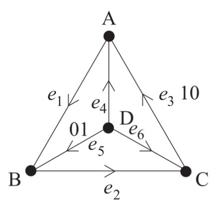
$$M = \begin{pmatrix} 1 & 1 & 2 & -1 & 0 & 1 \\ -1 & 1 & 0 & -1 & 2 & -1 \\ 1 & 1 & 0 & 1 & 0 & -1 \\ 1 & 0 & -1 & -1 & 0 & 0 \\ -1 & 1 & 0 & 0 & -1 & 0 \\ 0 & -1 & 1 & 0 & 0 & -1 \end{pmatrix}$$ and $b_1' \cdot b_1' = b_2' \cdot b_2' = 8$ and

$b_1' \cdot b_2' = 0$ shows that b_1', b_2' form the basis of a square lattice.

Embedding of the edges

$$M^{-1} \cdot \begin{pmatrix} 2 & 0 \\ 0 & 2 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} = \frac{1}{4} \begin{pmatrix} 1 & -1 \\ 1 & 1 \\ 2 & 0 \\ -1 & -1 \\ 0 & 2 \\ 1 & -1 \end{pmatrix}$$

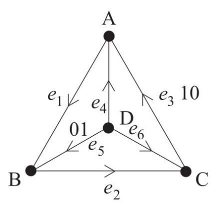
Determination of the vertices



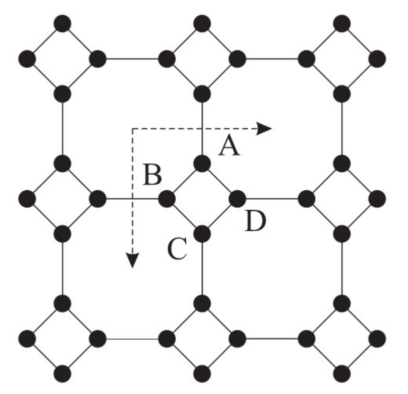
Choosing D at the origin, we obtain

$$\alpha(A) = \alpha(e_4) = \begin{pmatrix} -\frac{1}{4} & -\frac{1}{4} \end{pmatrix}$$
$$\alpha(B) = \alpha(e_1 + e_4) = \begin{pmatrix} 0 & -\frac{1}{2} \end{pmatrix}$$
$$\alpha(C) = \alpha(e_6) = \begin{pmatrix} \frac{1}{4} & -\frac{1}{4} \end{pmatrix}$$

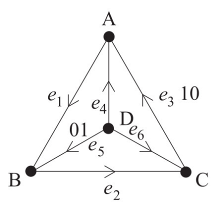
Embedding of 4.8^2



$$\alpha(A) = \begin{pmatrix} -\frac{1}{4} & -\frac{1}{4} \end{pmatrix}$$
$$\alpha(B) = \begin{pmatrix} 0 & -\frac{1}{2} \end{pmatrix}$$
$$\alpha(C) = \begin{pmatrix} \frac{1}{4} & -\frac{1}{4} \end{pmatrix}$$
$$\alpha(D) = \begin{pmatrix} 0 & 0 \end{pmatrix}$$



Determination of the point group type



Only those automorphisms of K_4 are admissible that map the kernel of the projection, spanned by $e_1 + e_2 + e_4 - e_6$, to itself.

$\sigma_1 = (A, B, C, D)$:

$e_3 - e_4 + e_6 \mapsto -e_1 - e_4 + e_5 \Rightarrow 10 \mapsto 01$

$-e_1 - e_4 + e_5 \mapsto -e_1 - e_2 - e_3 \Rightarrow 01 \mapsto \bar{1}0$

$\Rightarrow R(\sigma_1) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$ (4-fold rotation)

$\sigma_2 = (A, C)$:

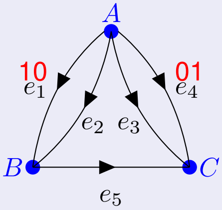
$e_3 - e_4 + e_6 \mapsto -e_3 + e_4 - e_6 \Rightarrow 10 \mapsto \bar{1}0$

$-e_1 - e_4 + e_5 \mapsto e_2 + e_5 - e_6 \Rightarrow 01 \mapsto 01$

$\Rightarrow R(\sigma_2) = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$ (reflection)

$\Rightarrow$ point group of type $4mm$.

Addendum to barycentric embedding exercise

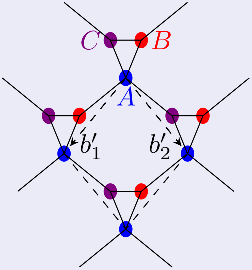


Zero voltage cycle $b_3 = \begin{pmatrix} 0 & 1 & -1 & 0 & 1 \end{pmatrix}$ is the kernel of the projection
$\Rightarrow$ basis cycles $b_1 = \begin{pmatrix} 1 & -1 & 0 & 0 & 0 \end{pmatrix}$ and $b_2 = \begin{pmatrix} 0 & 0 & -1 & 1 & 0 \end{pmatrix}$ have to be adjusted to become orthogonal to b_3.

$b_3 \cdot b_3 = 3$, $b_1 \cdot b_3 = -1$, $b_2 \cdot b_3 = 1$

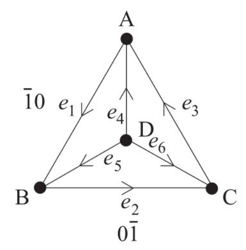
$$\Rightarrow b'_1 = 3b_1 + b_3 = \begin{pmatrix} 3 & -2 & -1 & 0 & 1 \end{pmatrix}$$
$$b'_2 = 3b_2 - b_3 = \begin{pmatrix} 0 & -1 & -2 & 3 & -1 \end{pmatrix}$$

$\Rightarrow$ centred rectangular lattice with $\measuredangle(b'_1, b'_2) \approx 78.5°$



Point group is of type pm, since only $(B, C)(e_1, e_4)(e_2, e_3)(e_5, -e_5)$ preserves the kernel of the projection.

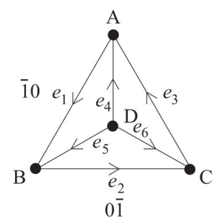
Exercise: Barycentric embedding by projection



For the voltage graph given above, determine a two-dimensional barycentric embedding.

- The direction of projection is determined by a cycle with zero voltage.
- To determine the type of the lattice, make sure to use a basis of the translation lattice that is orthogonal to the direction of projection.
- Also determine the type of the point group and of the plane group of this embedding.

Solution: Barycentric embedding by projection



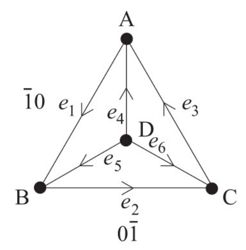
$$M = \begin{pmatrix} -1 & 0 & 0 & -1 & 1 & 0 \\ 0 & -1 & 0 & 0 & -1 & 1 \\ 0 & 0 & 1 & -1 & 0 & 1 \\ 1 & 0 & -1 & -1 & 0 & 0 \\ -1 & 1 & 0 & 0 & -1 & 0 \\ 0 & -1 & 1 & 0 & 0 & -1 \end{pmatrix}$$

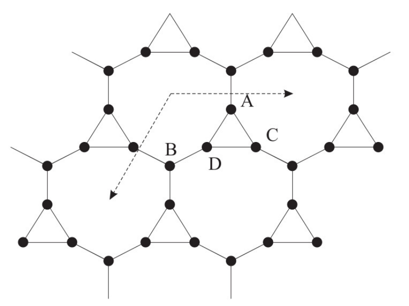
$$M^{-1} \cdot \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} = \frac{1}{4} \begin{pmatrix} -2 & -1 \\ -1 & -2 \\ -1 & -1 \\ -1 & 0 \\ 1 & -1 \\ 0 & 1 \end{pmatrix}$$

Choosing B at the origin gives
D at $\alpha(-e_5) = (-\frac{1}{4} \quad \frac{1}{4})$,
A at $\alpha(-e_5 + e_4) = (-\frac{1}{2} \quad \frac{1}{4})$,
B at $\alpha(-e_5 + e_6) = (-\frac{1}{4} \quad \frac{1}{2})$.

Solution: Barycentric embedding by projection (ctd.)

Adjusting the lattice basis: $b_3 \cdot b_3 = 3$, $b_1 \cdot b_3 = 1$, $b_2 \cdot b_3 = 1$
$\Rightarrow b_1' = 3b_1 - b_3$, $b_2' = 3b_2 - b_3$, $\measuredangle(b_1', b_2') = 120°$





$\sigma_1 = (A, D, C)$: $\begin{matrix} ADBA \mapsto DCBD \\ BDCB \mapsto BCAB \end{matrix} \Rightarrow R(\sigma_1) = \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}$

$\sigma_2 = (A, C)$: $\begin{matrix} ADBA \mapsto CDBC \\ BDCB \mapsto BDAB \end{matrix} \Rightarrow R(\sigma_2) = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$

Point group of type $3m$, plane group of type $p3m1$.