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A "Periodic Table" for Bravais Lattices

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lattice; **reduction**; **Delone**; **Selling**; **Delaunay**

Abstract

A convenient tabular display of the Bravais lattices types as defined by Delaunay (using Selling reduction) is described.

Note: In his later publications, Boris Delaunay used the Russian version of his surname, Delone.

1. stuff for larry to do

supplementary material – should there be a PDF file?/????

2. Introduction

Kahr (2023) suggested a "Periodic table of the space groups". In the same spirit, a "Periodic Table" of the Bravais lattice types is presented here. The table presents a systematic arrangement of the types, according to suggestions by Delaunay (1932). Like the periodic table of the elements, a brief amount of useful information is included.

3. The space $\mathbf{S^6}$

The scalars used by Delaunay (1932) in his formulation of Selling reduction (Selling, 1874) are (in the conventional order) $b \cdot c$, $a \cdot c$, $a \cdot b$, $a \cdot d$, $b \cdot d$, $c \cdot d$, where $d = -a - b - c$. (As a mnemonic device, observe that the first three terms use α, β, and γ, in that order, and the following terms use a, b, c, in that order.)

Andrews *et al.* (2019) chose to represent the Selling scalars in the space $\mathbf{S^6}$, $\{s_1, s_2, s_3, s_4, s_5, s_6\}$ (defined in the order above), as a way to create a metric space for the measurement of the distance between lattices.

4. The table

Delaunay (1932) and Delone *et al.* (1975) published a table of the Bravais types as distinguished by Selling (Delaunay) reduction.(Andrews & Bernstein, 2023) published a somewhat modified version of Delaunay's table. The table presented here in Fig. 1 is arranged with the lattice family types as columns and the Federov polyhedron types (Fedorov, 1891) (Fedorov, 1885) as rows.

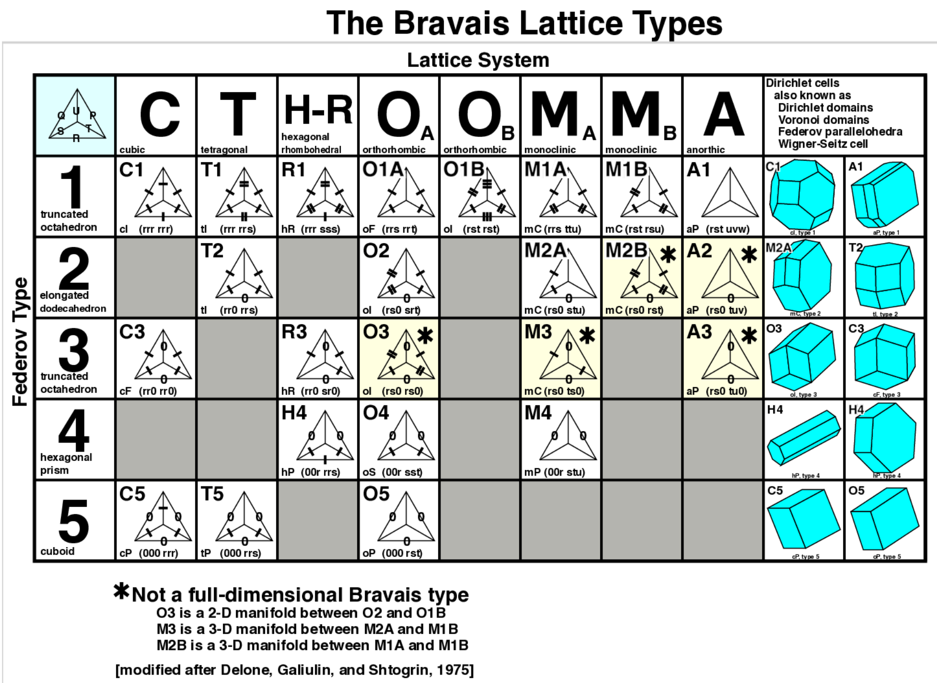

Fig. 1. The Bravais lattice types.

5. The labeling of the columns (lattice families)

The columns are labeled according to the lattice family: cubic, tetragonal, hexagonal-rhombohedral, orthorhombic, monoclinic, and triclinic (anorthic). The labels for each reflect the names: **C**, **T**, **H-R**, **O**, **M**, **A**, **H** (rather than the choices of Delaunay: **K**, **Q**, **R**, **O**, **M**, **T**, **H**, respectively).

In addition to combining the hexagonal and rhombohedral columns, a further change from the model of Delaunay is the splitting of orthorhombic and monoclinic into a pair of columns each ($\mathbf{O_A}$, $\mathbf{O_B}$, $\mathbf{M_A}$, $\mathbf{M_B}$). This change improved the display of these types. Delaunay had merged these disparate types into a single cell when their Federov types were identical. Thus, column **O** of Delaunay (1932) has become columns $\mathbf{O_A}$ and $\mathbf{O_B}$, etc.

6. The key cell (PQRSTU)

The International Tables for x-ray crystallography (von Laue, 1952) used the convention of labeling Selling parameters in the Bravais tetrahedron, as **P**, **Q**, **R**, **S**, **T**, **U**, corresponding to the $\mathbf{S^6}$ scalars $\{s_1, s_2, s_3, s_4, s_5, s_6\}$, respectively. For reference, the figure has been included in the upper left cell of the table. The values of the six Selling parameters given in the PQRSTU order unabiguously identify the cell and is called the "$\mathbf{S^6}$ characteristic" of the cell type, given at the bottom center of each cell of the table.. Note in particular which Selling parameters are zero, denoting right angles among them, and which ones are equal, denoting cases of higher symmetry.

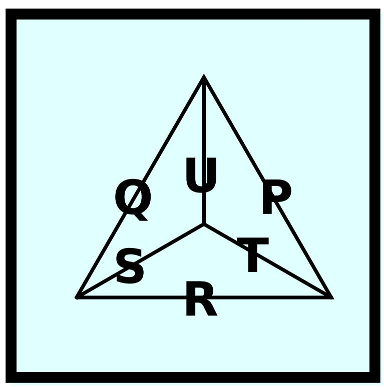

Fig. 2. The key cell with the labels used in the International Tables

7. The rows (Federov types)

Fedorov (1885) determined that there are only five kinds of parallelohedra that can be translated without rotations in 3-dimensional Euclidean space to fill space.

Except for rows 3 and 4, each row has a unique number of zero parameters. For rows 3 and 4, the difference is whether the two zeros are on opposite sides of the tetrahedron (type 3) or on adjacent sides (type 4). Type 3 is the case when the d-vector has a 90° angle to a, b, or c. Type 4 is the case where both 90° angles are among α, β, and γ.

8. The cells

In the table described here, the conditions for each Delone type are described using $\mathbf{S^6}$. For example, the cell for primitive cubic lattices is **C5**.

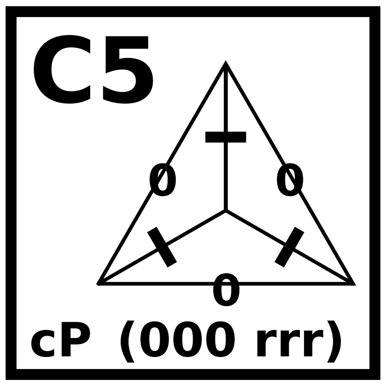

Fig. 3. The cell for the primitive cubic Bravais lattice type.

C5 is the label for the position (row and column, cubic and Federov type 5 reduced cell) within the table. The stylized tetrahedron shows which Selling parameters are zero or equal to each other. "cP" is the standard display for primitive cubic.

The $\mathbf{S^6}$ characteristic for that type is (000 rrr);

$s_1 = b \cdot c = 0$ ($\alpha = 90°$)

$s_2 = a \cdot c = 0$ ($\beta = 90°$)

$s_3 = a \cdot b = 0$ ($\gamma = 90°$)

$s_4 = s_5 = s_6$

9. Dirichlet cells

At the right end of the table, there are a few examples of Dirichlet cells for each row.

10. The unused/vacant cells

The cells shown in gray have no corresponding Bravais type.

11. Other changes from Delaunay

Within the table there are five cells that have a yellow background. Although Delaunay identified these among the 24 Bravais types, they are special in the sense that they do not possess the full dimensionality of their lattice family. Most likely, they are of only minor crystallographic interest.

Cells **A1** and **A2** are triclinic unit cells with one or two 90° angles. Respectively, they have only five or four free parameters.

O3 is a 2-D manifold that is the boundary between **O2** and **O1B**. With a characteristic of (rs0 rs0), **O3** has only two free parameters, not the three that are normal for an orthorhombic unit cell.

M3 is a 2-D manifold that is the boundary between **M1A** and **M1B**. With a characteristic of (rs0 ts0), **M3** has only three free parameters, not the four that are normal for an monoclinic unit cell.

There is a lack of unanimity in the crystallographic community on how best to present cells of the hexagonal-rhombohedral table cell in R1. In the table we follow the convention of (Burzlaff & Zimmermann, 1985) of using the hR (rrr sss) $\mathbf{S^6}$ lattice character (three equal cell edges and three equal cell angles $\neq 90°$). It is equally valid to choose settings to combine the R1 cells in threes to form true hexagonal H4 hP (00r rrs) super-cells with a and b as two equal edges with $\gamma = 120°$ and $\alpha = \beta = 90°$, and the original hidden pair of lattice points along body diagonals of the supercells.

12. Summary

13. Supplementary Material

The supplementary material includes the svg (Scalable Vector Graphics) file that generates the table.

Acknowledgements

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Synopsis

A tabular arrangement of the Bravais lattice types as defined by Delaunay is described.