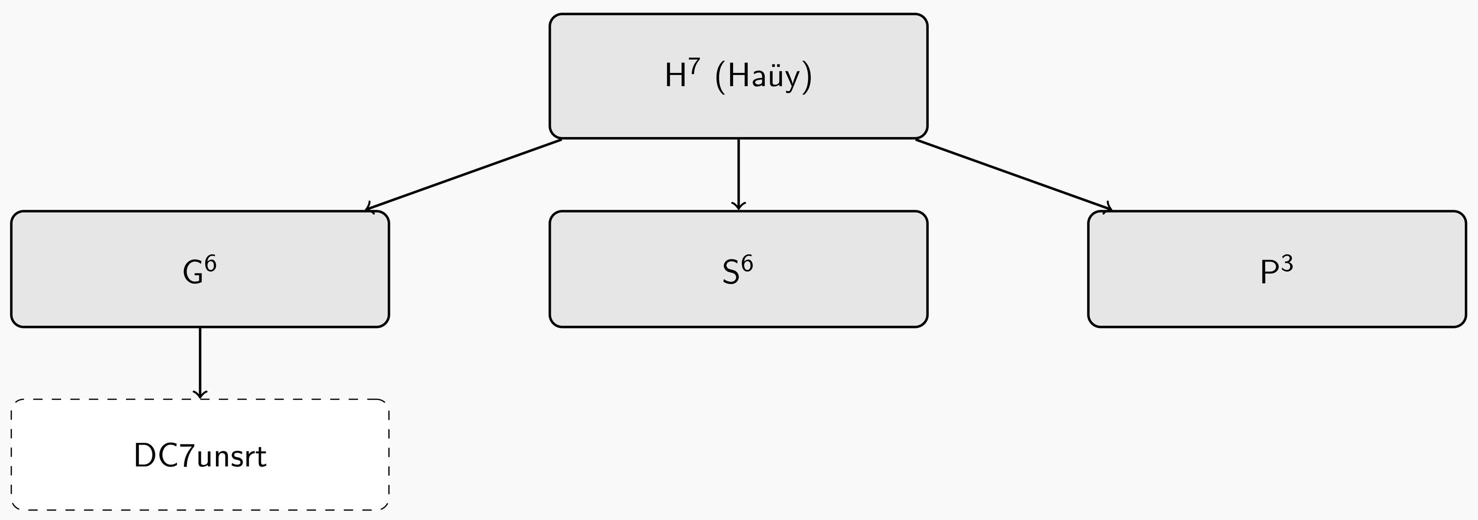
Unit Cells in Space or Spaces for Unit Cells

[0.5cm] Lawrence C. Andrews and Herbert J Bernstein — ACA 2025

Crystallographic Space Map



Abstract

Crystallographers describe unit cells using multiple mathematical spaces, each revealing different aspects of geometry, symmetry, or classification. But they don't think about them as spaces.
Beginning with conventional parameters in $\mathbf{H^6}$, we trace transformations through $\mathbf{G^6}$ and $\mathbf{S^6}$ into polar ($\mathbf{P^3}$), and geometric (DC7unsrt) spaces. Keep in mind that another common description is as the 3 base vectors of the conventional unit cell, $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$; this is also a space, a 3-dimensional space of 3-D Euclidiean vectors.

H^6 – Conventional Parameter Space

Conventional Parameter Space ($\mathbf{H^6}$)

Six coordinates: a, b, c, α, β, γ. Not ideal for comparing geometry or symmetry directly. ("H" was chosen to honor René Just Haüy, often described as the first modern crystallographer.)

C^3 – Character Space

Why do we need spaces for unit cells?

$\mathbf{H^6}$is inconvienent for describing the differences between unit cells/lattices, and there is no obvious method to display cells' relationships. Besides, other spaces are already in use; they are simply not always described as spaces. Representing cells as points in a space allows the simple application of the techniques of linear algebra.

S^6 – Selling/Delone Space

Delone Space ($\mathbf{S^6}$)

For a unit cell with base vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$, and -$\mathbf{d}$= -$\mathbf{a}$-$\mathbf{b}$-$\mathbf{c}$, a vector in $\mathbf{S^6}$ is defined as $[\mathbf{b}\cdot\mathbf{c},\ \mathbf{a}\cdot\mathbf{c},\ \mathbf{a}\cdot\mathbf{b},\ \mathbf{a}\cdot\mathbf{d},\ \mathbf{b}\cdot\mathbf{d},\ \mathbf{c}\cdot\mathbf{d}]$. In $\mathbf{S^6}$, the subspace of the Selling/Delaunay reduced points is a convex region. The Bravais types form linear manifolds. The region of the reduced vectors has only 6 boundaries, simplifying analyses.
$\mathbf{S^6}$is actually the space that Selling/Delaunay reduction is performed in.

G^6 – Niggli Space

Niggli Space (Metric Tensor Space) ($\mathbf{G^6}$))

For a unit cell with base vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$, a vector in $\mathbf{G^6}$ is defined as $[\mathbf{a}\cdot\mathbf{a},\ \mathbf{b}\cdot\mathbf{b},\ \mathbf{c}\cdot\mathbf{c},\ 2\mathbf{b}\cdot\mathbf{c},\ 2\mathbf{a}\cdot\mathbf{c},\ 2\mathbf{a}\cdot\mathbf{b}]$. $\mathbf{G^6}$is the basis for Niggli reduction. The domain of Niggli-reduced cells is non-convex with complex boundary behavior, so distance calculations can be done, but they can be complex.

DC7unsrt – Dirichlet 7 unsorted

Seven-Dimensional Dirichlet derived (DC7unsrt)

Seven scalars derived from Voronoi cells. Focuses on geometric relationships and symmetry inference. Bernstein, Andrews, and Xerri, Acta Cryst A79 (2005). 369-380. Experience shows that distance calculations in this space can be fast.

P^3 – Polar Space

Polar Space ($\mathbf{P^3}$)

$\mathbf{P^3}$is defined as the space of 3 polar coordinates, $[(|\mathbf{a}|,\alpha),(|\mathbf{b}|,\beta),(|\mathbf{c}\,\gamma)]$.
$\mathbf{P^3}$has a conceptual advantage that is it more directly related to the unit cell parameters that are commonly used in crystallography ($\mathbf{H^6}$). Polar coordinates are often converted to x,y, Euclidean coordinates for simple calculations with commensurate measures, so distance calculations make sense. Because they are in Angstrom units, they are more familar.