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$\mathbf{P^3}$, a simple metric for $\mathbf{H^6}$

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lattice; **unit cell**; **polar**; $\mathbf{P}^3$

Abstract

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

1. Introduction

In crystallography, cell geometry is conventionally encoded in a six-dimensional parameter space $\mathbf{H}^6 = (a, b, c, \alpha, \beta, \gamma)$.[1] But $\mathbf{H}^6$ is not a metric space (where distances can be simply defined), and $\mathbf{H}^6$ is not a vector space (where objects can be added and subtracted). In the same sense, symmetry operations have no simple representations in $\mathbf{H}^6$.

[1] "H" was chosen to honor early French crystallographer René Just Haüy.

For the above reasons, other spaces are often used to describe lattices, often for specialized purposes; see Table 1. Figure 1 shows relationships between several of these spaces. Although some of these spaces, such as $\mathbf{H}^6$ and $\mathbf{F}^3$ are in almost daily use, they are not often referred to as "spaces". In the case of $\mathbf{F}^3$, symmetry elements are linear operations in this space, and fractional coordinates of atomic positions are vectors expressed in this space.

Table 1. *Crystallographic spaces with their scalar definitions and analytical purposes*

Space	Scalars / Coordinates	Purpose
$\mathbf{H^6}$	a, b, $c \in \mathbb{R}_{>0}$ — edge lengths α, β, $\gamma \in (0°, 180°)$ — opposing angles Additionally, the sum of the angles must be less than 360° and must obey the triangle inequality	Composite parameter space described as $\mathbb{R}^3_{>0} \times (0°, 180°)^3$. The length dimensions are unconstrained, while the angles are geometrically restricted. Useful for conventional lattice descriptions, but limited in symmetry representation and metric-based classification.
$\mathbf{F^3}$	$\vec{a}$, $\vec{b}$, $\vec{c} \in \mathbb{R}^3$	Base vector space, a frame space (or frame bundle) in $\mathbb{R}^3$. The coordinates are the 3-space base vectors of a unit cell. Symmetry operations are enumerated using this space.
$\mathbf{P^3}$	$(\lvert\vec{a}\rvert, \alpha)$, $(\lvert\vec{b}\rvert, \beta)$, $(\lvert\vec{c}\rvert, \gamma)$ $\Rightarrow$ $(\lvert\vec{a}\rvert\cos\alpha,\ \lvert\vec{a}\rvert\sin\alpha$ $\lvert\vec{b}\rvert\cos\beta,\ \lvert\vec{b}\rvert\sin\beta$ $\lvert\vec{c}\rvert\cos\gamma,\ \lvert\vec{c}\rvert\sin\gamma)$ also known as: $(p1, p2, p3)$.	Polar coordinate space defined by the map $\mathbf{F}^3 \rightarrow \mathbf{P}^3$. Represents each base vector by magnitude and opposing angle, decomposed into directional components. Compact and smooth alternative to $\mathbf{H}^6$. $\mathbf{P}^3$ provides a simple and intuitive space for representing and comparing large numbers of unit cells. (This work)
$\mathbf{S^6}$	$s_1 = \vec{b}\cdot\vec{c}$, $s_2 = \vec{a}\cdot\vec{c}$, $s_3 = \vec{a}\cdot\vec{b}$ $s_4 = \vec{a}\cdot\vec{d}$, $s_5 = \vec{b}\cdot\vec{d}$, $s_6 = \vec{c}\cdot\vec{d}$ where $\vec{d} = -\vec{a} - \vec{b} - \vec{c}$	A space used for Selling/Delone reduction. The scalars are derived from dot products between lattice vectors. Used for lattice classification described by Delaunay and for distance computation (Andrews *et al.*, 2019). 24 Bravais types were defined by citeasnounDelone1975 in $\mathbf{S}^6$, but described using pictures showing the special relationships. Andrews & Bernstein (2023b) revised the table of Delone to include the $\mathbf{S}^6$vector definitions of the Bravais types.
$\mathbf{G^6}$	$g_1 = \vec{a}\cdot\vec{a}$, $g_2 = \vec{b}\cdot\vec{b}$, $g_3 = \vec{c}\cdot\vec{c}$ $g_4 = 2\vec{b}\cdot\vec{c}$, $g_5 = 2\vec{c}\cdot\vec{a}$, $g_6 = 2\vec{a}\cdot\vec{b}$	A space based on the metric tensor (and thus dot products of the basis vectors of the unit cell) and used for Niggli reduction and lattice distance computation. (Andrews & Bernstein, 2014) The International Tables for Crystallography describe the 44 Bravais types that result from Niggli reduction using algebraic expression in $\mathbf{G}^6$ (but stated in terms of scalars rather than manifolds in $\mathbf{G}^6$) (Aroyo, 2016).
$\mathbf{C}^3$	from the $\mathbf{S}^6$ scalars, $s1, ..., s6$ $c1 = (s1, s4), c2 = (s2, s5), c3 = (s3, s6)$ where (?,?) denotes a complex number	$\mathbf{C}^3$ was created to associate related scalars after the indication of Delone *et al.* (1975) concerning the "opposite" scalars in $\mathbf{S}^6$. Symmetry and Selling/Delaunay reduction have simpler forms in $\mathbf{C}^3$ than in $\mathbf{S}^6$. (Andrews & Bernstein, 2023a)
DC7u	d_1, d_2, d_3 — cell edge lengths d_4, d_5, d_6 — shorter face diagonals' lengths u — shortest body diagonal	Unsorted Dirichlet Cell space derived from Niggli-reduced cells. Defined by the map from lattice geometry to a 7-dimensional vector of distances. Fully invertible and smooth; used for rapid lattice distance computation. (Bernstein *et al.*, 2023)

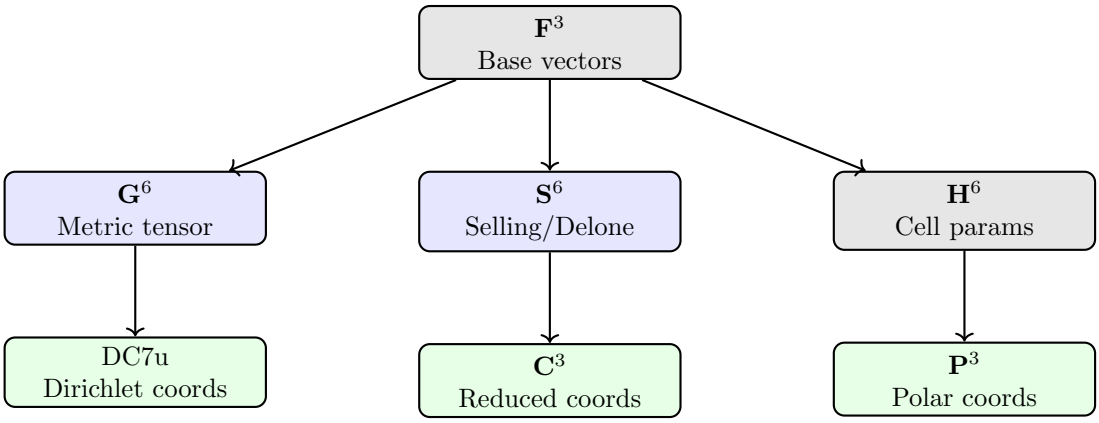

Fig. 1. Derived relationships among crystallographic spaces. Base vector space $\mathbf{F}^3$ gives rise to three scalar spaces: metric tensor space $\mathbf{G}^6$, Selling/Delone space $\mathbf{S}^6$, and conventional cell parameter space $\mathbf{H}^6$. Each transforms into a reduced or classification space: **DC7u** from $\mathbf{G}^6$, $\mathbf{C}^3$ from $\mathbf{S}^6$, and $\mathbf{P}^3$ from $\mathbf{H}^6$.

2. $\mathbf{P}^3$ Is introduced.

Delone *et al.* (1975) repeatedly pointed out the relationship of the "opposite" scalars in the tetrahedron representations of the Selling scalars. Examining those relationships show that the opposite terms are pairs where a term involving a is opposite a term involving α, etc.

Extending the observation of Delone *et al.* (1975), the idea occurs to make a triple of variables of those pairs. Since each pair has one length and one angle, we considered each pair as the definition of a polar coordinate space. The result is $\mathbf{P}^3$, a space of 3 2-dimensional polar coordinates. See Table 1 for the formal description. Two uses immediately are obvious.

The first uses the 2-dimensional character of the coordinates of $\mathbf{P}^3$. They allow simple to plot representations of collections of unit cells. See Figure 2, Figure 3, and Figure 4.

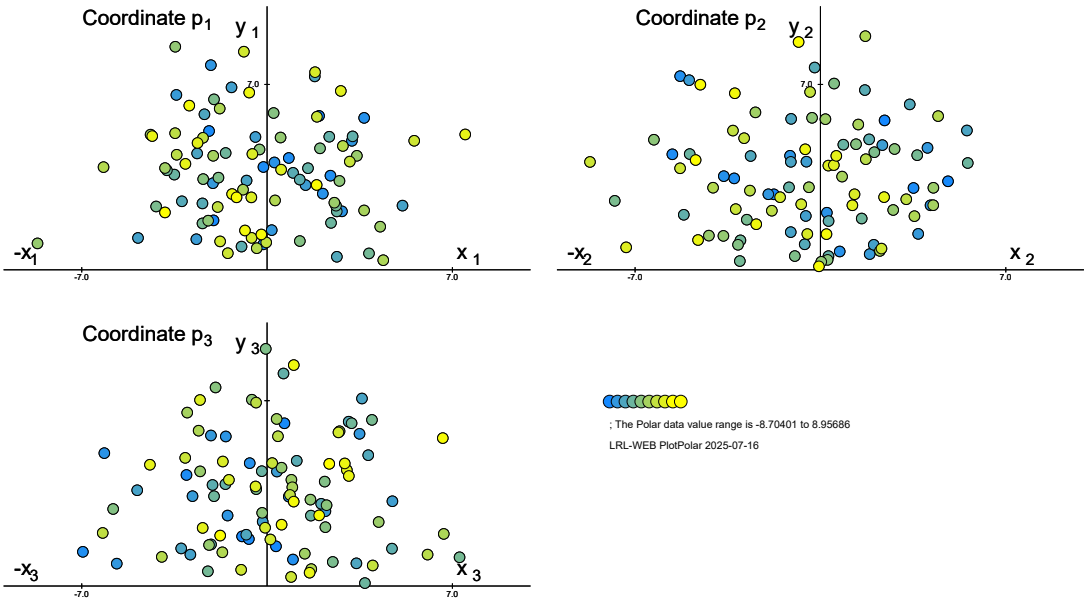

Fig. 2. 100 random primitive triclinic unit cells

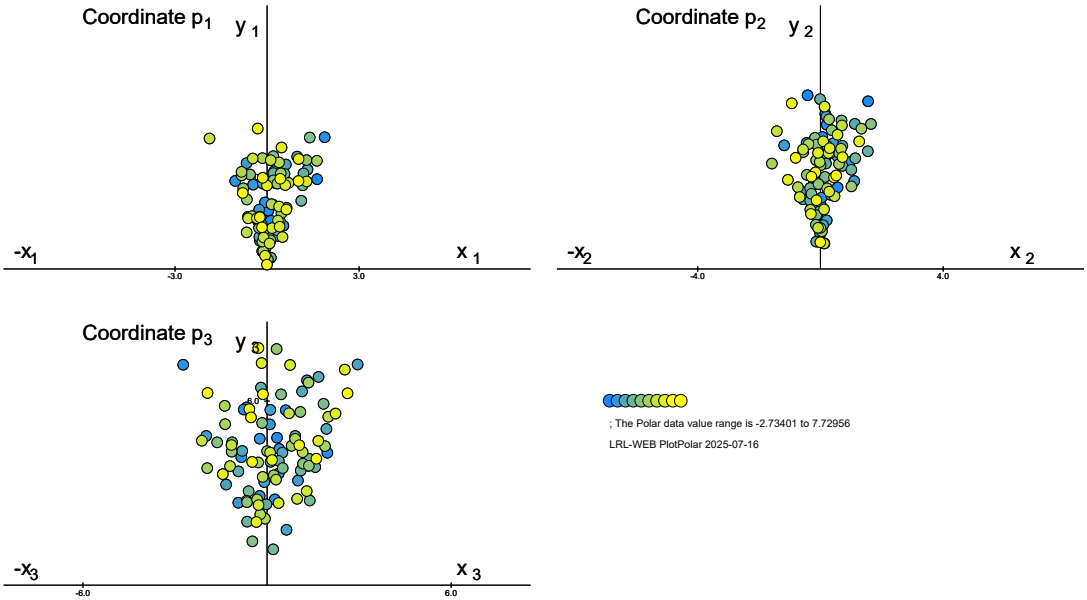

Fig. 3. The same100 random primitive triclinic unit cells, Niggli-reduced

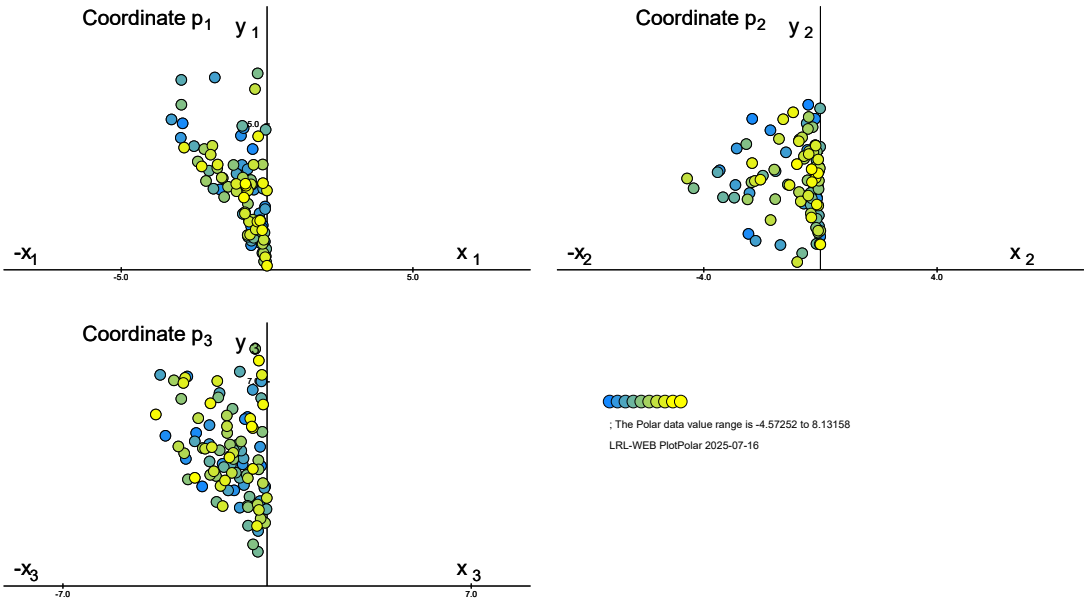

Fig. 4. The same 100 random primitive triclinic unit cells, Selling-reduced

The second use is allowing the calculation of Euclidean distances. Because $\mathbf{P}^3$ can be represented as 3 xy planes, the Euclidean difference between any two unit cells described as $\mathbf{P}^3$ can be easily computed. Thus use contrasts with $\mathbf{H}^6$, where incommensurate lengths and angles do not lend themselves to a distance calculation.

3. Relationship to Other Spaces

While derived from the same foundational cell parameters as $\mathbf{H^6}$, the space $\mathbf{P^3}$ sidesteps issues of angular nonlinearity that arise in conventional cell representations. Compared with $\mathbf{C^3}$, which seeks symmetry-reduced coordinates derived from $\mathbf{S^6}$, the construction of $\mathbf{P^3}$ is more geometric than algebraic. It provides a useful intermediary: more interpretable than metric tensors or other spaces, less abstract than $\mathbf{S}^6$ or $\mathbf{G}^6$.

4. Notation

5. Matrices of boundary transformations

5.1. Derivation

5.2. Example P++ implementation

5.3. Example of use

6. Graphical display of projections

7. Scalar Reduction and Canonical Presentation in Projected Vector Triplets

7.1. 1. Standard Presentation of Projected Vectors

Let a set of three projected vectors be given:

$$(p_1, p_2, p_3), \quad p_i \in \mathbb{R}^2$$

Each p_i is constructed from a lattice vector via magnitude and opposing angle:

$$p_i = |\vec{v}_i|(\cos\theta_i, \sin\theta_i)$$

The **Standard Presentation** algorithm assigns a canonical ordering and orientation to the triplet:

1. **Magnitude Sort:** Reorder vectors so that

   $$|p_1| \leq |p_2| \leq |p_3|$$

   using Euclidean norms $|p_i| = \sqrt{x_i^2 + y_i^2}$. Ties are preserved up to a numerical tolerance δ.

2. **Directional Coherence:** If the x-components of the triplet are not all of consistent sign, flip the necessary vectors by negating only the x_i component:

$$p_i \to (-x_i,\ y_i)$$

This maps quadrant I vectors into quadrant II, preserving their placement in the upper half-plane and maintaining angular conventions typical in crystallographic analysis.

$$p_i \to (-x_i,\ -y_i)$$

to align the triplet into a directionally consistent state. If all $x_i < 0$, the configuration is already coherent and requires no change.

$$p_i \to (-x_i, -y_i)$$

for any two vectors, preserving chirality.

3. **Return Ordered Triplet:** Output the permuted and flipped triplet with consistent magnitude order and cosine directionality.

7.2. 2. Scalar Projection Interaction and Cost Function

For any pair of projected vectors $p_i, p_j \in \mathbb{R}^2$, define the scalar projection interaction (or directional affinity):

$$\mu_{ij} = p_i \cdot p_j = x_i x_j + y_i y_j$$

The **scalar coupling cost** is then defined over the triplet as:

$$C' = \frac{|\mu_{12}| + |\mu_{13}| + |\mu_{23}|}{p_1 \cdot p_1 + p_2 \cdot p_2 + p_3 \cdot p_3}$$

This cost measures the normalized sum of pairwise directional alignment. Lower values of C' indicate that the projected vectors are less directionally coupled — i.e., more orthogonal or dispersed.

7.3. 3. Scalar Reduction Algorithm

The goal of scalar reduction is to transform the triplet (p_1, p_2, p_3) into an algebraically simpler form — one with lower scalar coupling cost C' — while preserving lattice identity (e.g., volume and reconstructability).

The reduction proceeds iteratively:

1. **Initialization:** Apply standard presentation. Compute initial cost C'_0 and physical volume $V_0 > 0$.

2. **Pairwise Projection Subtractions:** For each unordered pair $(p_i, p_j),\ i \neq j$, compute the scalar coefficient:

   $$\lambda = \frac{p_i \cdot p_j}{p_j \cdot p_j}$$

   Then define the candidate vector:

   $$p'_i = p_i - \lambda p_j$$

3. **Evaluate Candidate:** Apply standard presentation to updated triplet. Recompute cost C'_{new} and volume V_{new}.

4. **Acceptance Criteria:** Accept the transformation if:

$$C'_{\text{new}} + \delta < C' \quad \text{and} \quad V_{\text{new}} > 0$$

5. **Repeat:** Continue until no further accepted transformations lower the cost.

6. **Output:** Return the reduced triplet $(p_1, p_2, p_3)_{\text{red}}$ with minimal scalar cost.

7.4. 4. Interpretation of Cost and Reduction

The term "reduction" refers to minimizing the scalar coupling among vectors — reducing directional alignment that obscures presentation clarity. The cost C' is a rigorously defined metric for this alignment. Transformations reduce C' while preserving:

- The vector magnitudes and their reconstructable relationships
- The unit cell's volume and crystallographic identity
- The triplet's algebraic validity in scalar projection space

Reduction leads to a cleaner, more canonical representation of the original structure — just as Niggli reduction provides a minimal cell in metric tensor space, scalar reduction provides a minimal configuration in projected vector space.

8. Summary

9. Availability of code

CmdToP3 and PlotPolar are available in github.com, in `https://github.com/duck10/LatticeRepLib.git`.

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Synopsis