January 19, 2026

$\mathbf{P^3}$, linearizing unit cell parameters

Lawrence C. Andrews[a]* and Herbert J. Bernstein[a]

[a]*Ronin Institute for Independent Scholarship 2.0, USA.*

E-mail: larry6640995@gmail.com

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

Abstract

The space $\mathbf{P}^3$ is introduced, derived from unit cell axial lengths and interaxial angles. $\mathbf{P}^3$ enables linearization of unit cell parameters using three polar coordinate bases.

$\mathbf{P}^3$ serves as a compact, interpretable alternative to more abstract spaces such as $\mathbf{G}^6$ and $\mathbf{S}^6$.

1. Introduction

In crystallography, unit cell geometry is conventionally encoded in a six-dimensional parameter space $\mathbf{H}^6 = (a, b, c, \alpha, \beta, \gamma)$.[1] However, $\mathbf{H}^6$ is not a metric space (where distances can be simply defined), nor is $\mathbf{H}^6$ a vector space (where objects can be added and subtracted). In the same sense, symmetry operations have no simple representations in $\mathbf{H}^6$. In consequence, $\mathbf{H}^6$ has no simple measure of the "difference" between

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

two lattices; how can one compare a difference of 1 Ångstrom unit vs. one angular degree?

[*Note: Boris Delaunay in his later publications chose to render his surname as "Delone" (which is still pronounced the same as Delaunay).*]

For the above reasons, other spaces are often used to describe lattices, often for specialized purposes; see Table 1. Figure 1 shows relationships among 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.

We propose a "linearized" space, $\mathbf{P}^3$, derived from $\mathbf{H}^6$, but having all measures in Ångstrom units (or other chosen linear measures.)

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	Composite geometric parameter space $\mathbb{R}^3_{>0} \times (0°, 180°)^3$. Lengths are unconstrained; angles are geometrically restricted. The angles must obey the spherical triangle inequalities (summing to less than 360 degrees, and the sum of any 2 must not exceed the third). $\mathbf{H}^6$ is 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 in $\mathbb{R}^3$. Coordinates are the three-space base vectors of a unit cell. Lattices are defined using the components of $\mathbf{F}^3$, and translational symmetry is described in $\mathbf{F}^3$.

Continued on next page

Table 1 continued

Space	Scalars / Coordinates	Purpose
$\mathbf{B}^4$	$\vec{a}$, $\vec{b}$, $\vec{c}$, $(-\vec{a}-\vec{b}-\vec{c})$ in $\mathbb{R}^3$	Base vector space in $\mathbf{F}^3$ plus the negative sum of the three base vectors. This set of vectors is used in the definition of $\mathbf{S}^6$, which is the space of Selling/Delone reduction.
$\mathbf{P}^3$	$(\lvert\vec{a}\rvert, \alpha)$, $(\lvert\vec{b}\rvert, \beta)$, $(\lvert\vec{c}\rvert, \gamma)$ $\Rightarrow$ $(\lvert\vec{a}\rvert\cos\alpha,\ \lvert\vec{a}\rvert\sin\alpha)$ $(\lvert\vec{b}\rvert\cos\beta,\ \lvert\vec{b}\rvert\sin\beta)$ $(\lvert\vec{c}\rvert\cos\gamma,\ \lvert\vec{c}\rvert\sin\gamma)$ also known as (p_1, p_2, p_3)	Polar coordinate space defined in terms of unit cell axial lengths and their opposing angles (opposing, the angle between the other two unit cell axes). It is a compact and smooth alternative to $\mathbf{H}^6$. Useful for comparing 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 $\vec{d} = -\vec{a}-\vec{b}-\vec{c}$	Used for Selling/Delone reduction. The scalar components are dot products between lattice vectors. $\mathbf{S}^6$ supports Bravais lattice classification. 24 Bravais types were defined using the scalar components of $\mathbf{S}^6$ by Delone (1975), later revised using $\mathbf{S}^6$ (Andrews & Bernstein, 2023*b*).
$\mathbf{G}^6$	$g_1 = \vec{a}\cdot\vec{a}$, $g_2 = \vec{b}\cdot\vec{b}$, $g_3 = \vec{c}\cdot\vec{c}$ $g_4 = 2\vec{b}\cdot\vec{c}$, $g_5 = 2\vec{c}\cdot\vec{a}$, $g_6 = 2\vec{a}\cdot\vec{b}$	$\mathbf{G}^6$ is based on the metric tensor and used for Niggli reduction and lattice distance computation (Andrews & Bernstein, 2014). The International Tables describe 44 Bravais types using scalar expressions derived from $\mathbf{G}^6$ (Aroyo, 2016).
$\mathbf{C}^3$	From $\mathbf{S}^6$ scalars: $s_1, \ldots, s_6$ $c_1 = (s_1, s_4)$, $c_2 = (s_2, s_5)$, $c_3 = (s_3, s_6)$ where the parentheses denote a complex number	$\mathbf{C}^3$ associates scalar pairs identified by Delone as "opposites." Symmetry and Selling/Delone reduction simplify in this space (Andrews & Bernstein, 2023*a*).
DC7u	d_1, d_2, d_3 — edge lengths d_4, d_5, d_6 — shortest face diagonals u — shortest body diagonal	**DC7u**: unsorted Dirichlet Cell space derived from Niggli-reduced cells. Defined as a 7D vector of distances. Fully invertible and smooth; used for rapid lattice distance computation (Bernstein *et al.*, 2023).

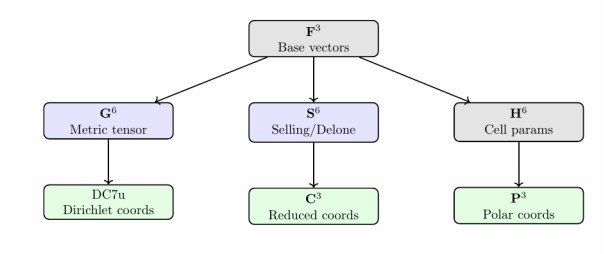

Fig. 1. Schematic relationships among crystallographic spaces. The base vector space $\mathbf{F}^3$ gives rise to three scalar spaces: metric tensor space $\mathbf{G}^6$, Selling/Delone space $\mathbf{S}^6$, and conventional cell parameter space $\mathbf{H}^6$. Each transforms into a reduced or classification 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 shows that the opposite terms are pairs where a term involving **a** is opposite a term involving α, *etc.*

As described in Table 1, the Selling scalars are a vector: $[s_1, s_2, s_3, s_4, s_5, s_6]$. Delaunay (1933) represents their relationships as the edge components of a tetrahedron as shown in Figure 2.

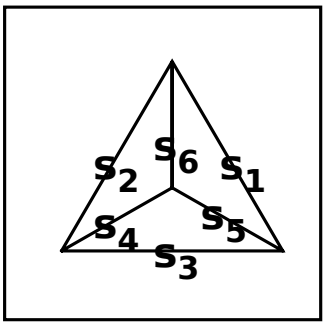

Fig. 2. The relationships of the Selling scalars as described by Delaunay (1933), but labeled using the vector components of $\mathbf{S}^6$ (Andrews & Bernstein, 2023*b*). Visualized as a 3 dimensional tetrahedron, scalar s_1 is opposite scalar s_4, etc. The number of each scalar is the position in the $\mathbf{S}^6$ vector. See Table 1 for the definitions of the scalars in space $\mathbf{S}^6$.

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

The first use applies the two-dimensional character of the coordinates of $\mathbf{P}^3$. They allow simple-to-plot representations of collections of unit cells. Plotting each of the coordinates of $\mathbf{P}^3$ generates plots that are easily interpreted as crystallographic axial length/opposite angle pairs. The distance of a point from the origin has a length equal to the axial length, and the interaxial angle between the 2 other bases (plotted as the angle from the x-axis) is illustrated on the plots. Basically, together the three plots of the three coordinates are simple projections of $\mathbf{H}^6$. See Section 4.

A second use is allowing the calculation of Euclidean distances between pairs of unit cells. Because $\mathbf{P}^3$ can be represented as three xy planes, the Euclidean difference between any two unit cells described as $\mathbf{P}^3$ can be easily computed. This use contrasts with $\mathbf{H}^6$, where incommensurate lengths and angles do not lend themselves to a distance calculation. See Section 5.

3. Relationship to Other Spaces

While $\mathbf{P}^3$ is derived from the same foundational cell parameters as $\mathbf{H^6}$, $\mathbf{P^3}$ sidesteps issues of angular nonlinearity that arise in the conventional cell representation. Compared with $\mathbf{C^3}$ (Andrews & Bernstein, 2023*a*), which derives coordinates 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, but less abstract than $\mathbf{S}^6$ or $\mathbf{G}^6$.

4. Graphical display of projections

$\mathbf{P}^3$ allows simple-to-plot representations of collections of unit cells. See Figures 3, 4, and 5, where 100 randomly chosen triclinic cells are plotted (Figure 3), and the effects of unit cell reduction are demonstrated (Figure 4 and Figure 5).

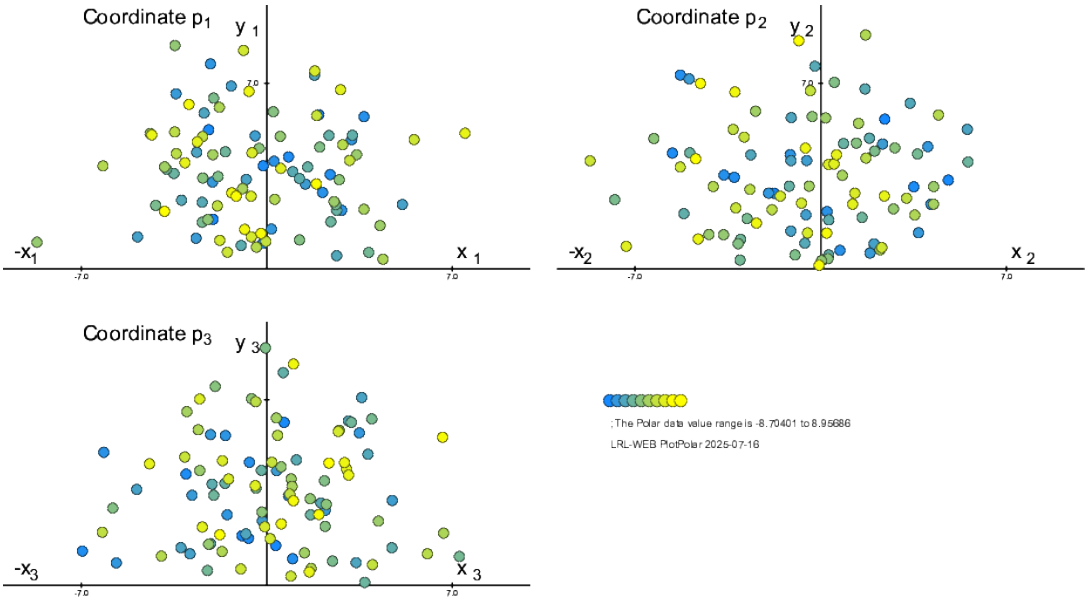

Fig. 3. Scatter plots of 100 randomly selected primitive triclinic unit cells represented in $\mathbf{P}^3$. Each of the 3 components of $\mathbf{P}^3$ is shown. (Colors reflect the order of input of the unit cells.)

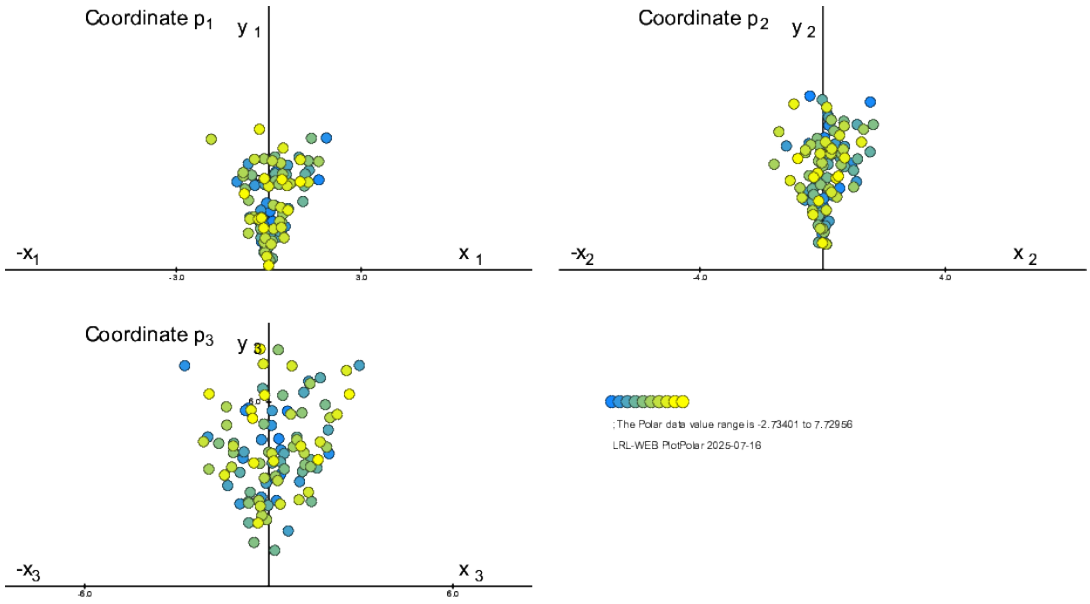

Fig. 4. Scatter plots of the same 100 randomly selected primitive triclinic unit cells represented in P3 as shown in Figure 3, Niggli-reduced.

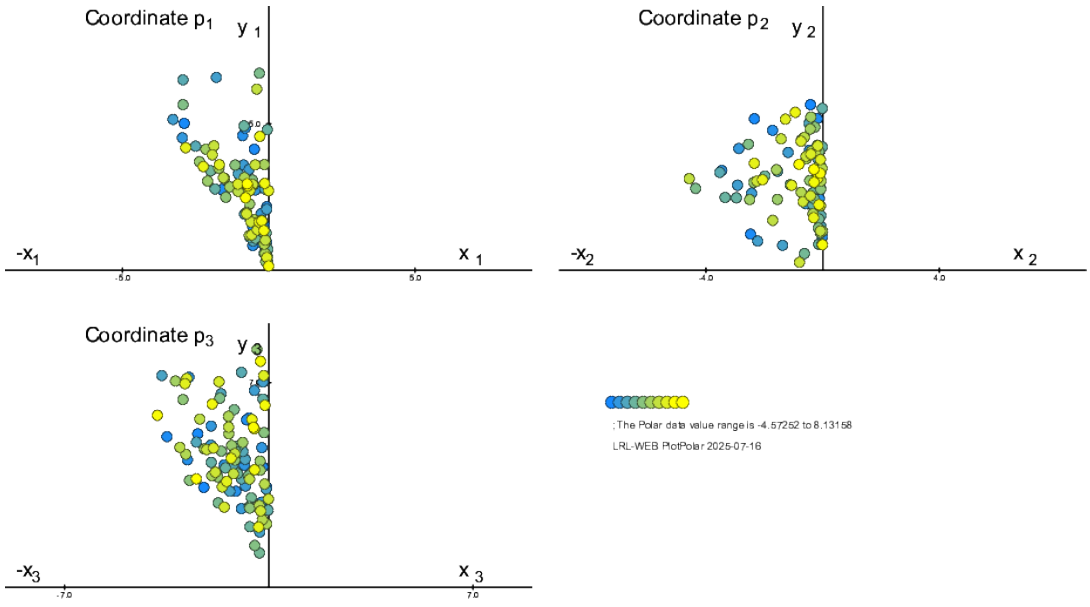

Fig. 5. Scatter plots of the same 100 randomly selected primitive triclinic unit cells represented in $\mathbf{P}^3$ as shown in Figure 3, Selling/Delone-reduced.

5. Comparing different unit cells

In 3-space, measuring the Euclidean distance between two points is just computing the square root of the sum of the squares of the differences in the three coordinates. Similarly in $\mathbf{P}^3$, we compute distances from the square root of the sum of squared differences between the three polar coordinates. Polar coordinates have a Euclidean measure from their xy representation. So, taking the 6 scalar values of 2 unit cells presented in $\mathbf{P}^3$, we calculate a Euclidean distance by the ordinary method.

Let us compare two cells derived by modifying a primitive unit cell to form two slightly modified cells, one by changing γ, and one by changing $\vec{c}$.

1. P 10 10 10 90 90 90
2. P 10 10 10 90 90 91
3. P 10 10 10.1 90 90 90

The Euclidean distances between these cells are:

- 1–2: 0.175
- 1–3: 0.100
- 2–3: 0.202

In this example, a 1.0° change in γ yields a Euclidean distance comparable to a 0.1 Å change in the c-axis length.

6. Summary

The space $\mathbf{P}^3$ is introduced. Less abstract than spaces based on dot products and metric tensors, it provides a simple way to understand the method for comparing unit cells and a convenient method of displaying unit cells.

7. Availability of code

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

Acknowledgements

Careful copy-editing and corrections by Frances C. Bernstein are gratefully acknowledged.

Funding information

Funding for this research was provided in part by: U.S. Department of Energy Offices of Biological and Environmental Research and of Basic Energy Sciences (grant No. DE-AC02-98CH10886; grant No. E-SC0012704); U.S. National Institutes of Health (grant No. P41RR012408; grant No. P41GM103473; grant No. P41GM111244; grant No. R01GM117126, grant No. 1R21GM129570); Dectris, Ltd.

8. Synopsis

$\mathbf{P}^3$ is a linearized description of unit cell parameters, created from the usual lengths and angles of the unit cell. It provides a useful metric for comparing unit cells and a convenient base for displaying and comparing unit cells.

References

Andrews, L. C. & Bernstein, H. J. (2014). *J. Appl. Cryst.* **47**(1), 346 – 359.

Andrews, L. C. & Bernstein, H. J. (2023*a*). *Acta Cryst.* A**79**(5), 499–503.

Andrews, L. C. & Bernstein, H. J. (2023*b*). *Acta Cryst.* A**79**(5), 485–498.

Aroyo, M. I. (ed.) (2016). *International Tables for Crystallography, Volume A: Space-Group Symmetry*. International Union of Crystallography, second online edition ed. **URL:** *https://it.iucr.org/A/*

Bernstein, H. J., Andrews, L. C. & Xerri, M. (2023). *Acta Cryst.* A**79**(4), 369–380.

Delaunay, B. N. (1933). *Z. Krist.* **84**, 109 – 149.

Delone, B. N., Galiulin, R. V. & Shtogrin, M. I. (1975). *J. Sov. Math.* **4**(1), 79 – 156.