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

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Abstract

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

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

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

3. Scalar Reduction and Canonical Presentation in Projected Vector Triplets

3.1. 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.

3.2. 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.

3.3. 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.

3.4. 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.

4. Summary

5. Availability of code

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

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Synopsis