

August 17, 2023

What are unit cells

LAWRENCE C. ANDREWS^{a*} AND HERBERT J. BERNSTEIN^b

^a*Ronin Institute, 9515 NE 137th St, Kirkland, WA, 98034-1820 USA, and* ^b*Ronin Institute, c/o NSLS-II, Brookhaven National Laboratory, Upton, NY, 11973 USA.*

E-mail: larry6640995@gmail.com

lattice; unit cells; Delone; Selling

Abstract

Abstract Unit cells

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

1. Introduction

The term “unit cell” is now the most commonly used term for a smallest repeating unit of a crystal structure. It allows us to describe the crystal structure in terms of a simple geometric shape. This makes it easier to visualize the structure and to calculate its properties.

2. Conventional 3-space methods

2.1. Lattices as basis vectors

The fundamental understanding of crystals begins from the study of lattices. A typical lattice Λ in \mathbb{R}^n thus has the form

$$\Lambda = \left\{ \sum_{i=1}^n a_i \mathbf{v}_i \mid a_i \in \mathbb{Z} \right\},$$

where: $(\mathbf{v}_1, \dots, \mathbf{v}_n)$ is a basis of the lattice. Conventionally, "the unit cell" is defined as the set of n vectors generated by $a_i = 1$.

In crystallography, we study the lattice in three-dimensional space ($n=3$ in the above equation). We use 3×3 matrices to create different unit cells by manipulating a vector of 3D vectors. These manipulations are usually described as happening in 3D space, but the vector of 3D vectors is actually a mathematical object with nine parameters in a space that can be described as $R^3 x R^3$, which is a nine-dimensional space.

2.2. $a, b, c, \alpha, \beta, \gamma$

The second conventional representation of unit cells is 2 triplets: 3 edge lengths of the basis vectors and the 3 angles between them. This is a 6-dimensional space: $R^3 x R^3$.

The problem with this representation occurs in the cases where the need is to compare two (or more) unit cells. The representation as $R^3 x R^3$ informs us that the two R^3 are not necessarily commensurate. Indeed, the edge lengths and the interaxial angles have no shared measure. (However, see Section 2.3.)

2.3. Polar coordinates

Section 2.2 alluded to the incommensurate nature of the two subspace of $R^3 x R^3$.

Delone et al. (1975) commented on the importance of the "opposite" scalars in the Bravais tetrahedron. Andrews et al. (2019) observed that the association of those

opposites implied the association of each unit cell edge with the opposite interaxial angle:

$$(a, \alpha), (b, \beta), (c, \gamma).$$

They used that association to create a space C^3 (see Section 4.2). Using the above definition (2.3, we can define a 6-dimensional space P^3 . Unlike the issue with the direct use of lengths and angles, polar coordinates are a well-known 2-dimensional object with the alternative representation as (x, y) , the 2-dimensional plane, where we can immediately use Euclidean distance measure.

2.4. Dirac

Dirac cells are defined as one or more primitive unit cell between a pair of lattice plans. Physicists use Dirac cell in the computation of energy levels (Dirac, 1930).

3. Niggli space

4. Delone space

4.1. S^6

4.2. C^3

4.3. Root Invariant

5. Wigner-Seitz space

6. Notation

7. Summary

Summary unit cells

8. Availability of code

The C^{++} code for C^3 and related software tools is available in github.com, in <https://github.com/duck10/LatticeRepLib.git>. The program CmdToC3 uses the required files.

Acknowledgements

Careful copy-editing and corrections by Frances C. Bernstein are gratefully acknowledged. Our thanks to Jean Jakoncic and Alexei Soares for helpful conversations and access to data and facilities at Brookhaven National Laboratory.

Funding information

Funding for this research was provided in part by: US 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.

References

- Andrews, L. C., Bernstein, H. J. & Sauter, N. K. (2019). *Acta Cryst.* **A75**(3), 593–599.
 Bragg, W. H. & Bragg, W. L. (1915). X rays and crystal structure. Bell.
 Delone, B. N., Galiulin, R. V. & Shtogrin, M. I. (1975). *J. Sov. Math.* **4**(1), 79 – 156.
 Dirac, P. A. M. (1930). The principles of quantum mechanics. Oxford University Press.

Synopsis

Unit cells
