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Unit cells considered in polar coordinates

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abstract

1. Introduction

The representation of the crystal lattice parameters as a , b , c , α , β , and γ dates from early in the 20th century. The association that a is opposite to α , etc. is at least that old.

Delone *et al.* (1975) emphasized the relationship of the "opposite" Selling scalars in the Bravais tetrahedron representation of lattice.

Andrews *et al.* (2019) took the association one step farther, combining the "opposite" pairs of the 6 Selling scalars into the 3 complex coordinates.

The above ideas are here carried to another representation of lattice parameters. Taking the concept that the dimension a is related to the angle α , etc. those pairs are considered to be 3 points represented in polar coordinates: (a, α) , (b, β) , and (c, γ) .

2. Notation

ZZZZZZZZZZZZZZZZZZ

3. Summary

XXXXXXXXXXXXXXXXXXXX

4. Availability of code

The C++ code for **C³** and related software tools is available in [github.com](https://github.com/duck10/LatticeRepLib.git), in <https://github.com/duck10/LatticeRepLib.git>. The program Radial uses the required files.

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References

- Andrews, L. C., Bernstein, H. J. & Sauter, N. K. (2019). *Acta Cryst.* **A75**(3), 593 – 599.
- Delone, B. N., Galiulin, R. V. & Shtogrin, M. I. (1975). *J. Sov. Math.* **4**(1), 79 – 156.