

Crystal Symmetry Primer*

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February 25, 2023

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0 Preliminary

0.1 Recommended books and lecture notes

0.2 International table for crystallography

0.3 Spglib

1 Symmetry operation and space group

1.1 Symmetry operation, isometry

1.2 Affine group, Euclidean group

1.3 Matrix-column pair, Setiz symbol, augmented matrix, short-hand notation

Note: hexagonal axis for $p3$

1.4 Screw and glide

1.5 Working example from plane group

2 Group theory primer

2.1 Definition

2.2 Abelian group

translation subgroup

2.3 Isomorphism, subgroup

2.4 Coset decomposition, normal subgroup, factor group

\mathbb{Z}_2 in \mathbb{Z}_4

2.5 Homomorphism, kernel, image

point group

2.6 Conjugation

3 Group structure of space groups

3.1 Definition of space group

3.2 Point group

3.3 Vector system

symmorphic and nonsymmorphic space groups

3.4 Working example from plane group

4 Classification of space groups

4.1 Transformation matrix, origin shift

4.2 219 affine space-group types

4.3 230 space-group types

11 enantiomorphic pairs

4.4 32 geometric crystal classes

4.5 14 Bravais types of lattices

limiting case

special metric

4.6 7 crystal systems

4.7 73 arithmetic crystal classes

5 Conventions for space groups

5.1 Conventional cell

5.2 Hermann–Mauguin symbol

Principal directions

How to read H-M symbols

5.3 Standard settings in ITA

5.4 Hall symbol

6 Magnetic space group

6.1 Definition

6.2 BNS and OG symbols

6.3 Construction type of magnetic space group

6.4 Magnetic Hall symbol

7 Site symmetry group and normalizer

7.1 Action, orbit, stabilizer

7.2 Site symmetry group, Wyckoff position, asymmetric unit

7.3 Euclidean normalizer

7.4 Wyckoff set, equivalent descriptions of crystal structure

7.5 Affine normalizer

8 Lattice computation

8.1 Delaunay reduction

8.2 Choice of basis vectors, sublattice

8.3 Hermite normal form

8.4 Smith normal form

References