Computational Solid State Physics, part II

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Lab1: Crystal Structure and Symmetry:

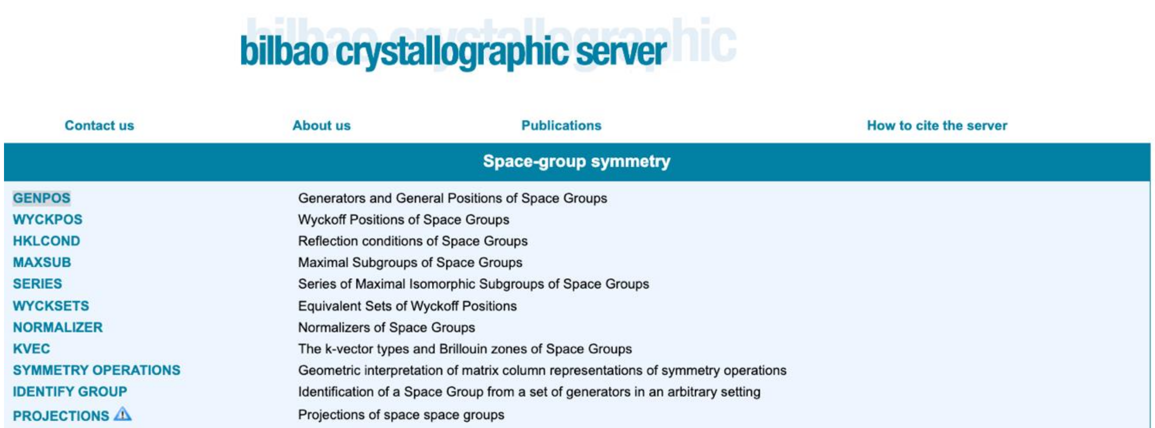
- **What is a Crystal Structure?** Lattice, Unit cells, Bravais lattices, etc.
- **Symmetry in Crystals:** Types of Symmetry operations, Point Groups, Space Groups.
- **Space Groups:** Definition, Notations – International Tables of Crystallography.
- **Wyckoff Positions:** Definition of Wyckoff Positions.
- Using the **Bilbao Crystallographic Server -** https://www.cryst.ehu.es/
- **Setting up and visualizing simple and complex crystal structures with VESTA:** https://jp-minerals.org/vesta/en/

Lab1: Tools & References

Crystal Structure Visualization (VESTA):

Download **VESTA** from: https://jp-minerals.org/vesta/en/ (Linux, Windows and Mac versions); Install following the installation instructions on the website.

Interactive Crystallographic Table (Bilbao Crystallographic Server):



bilbao crystallographic server

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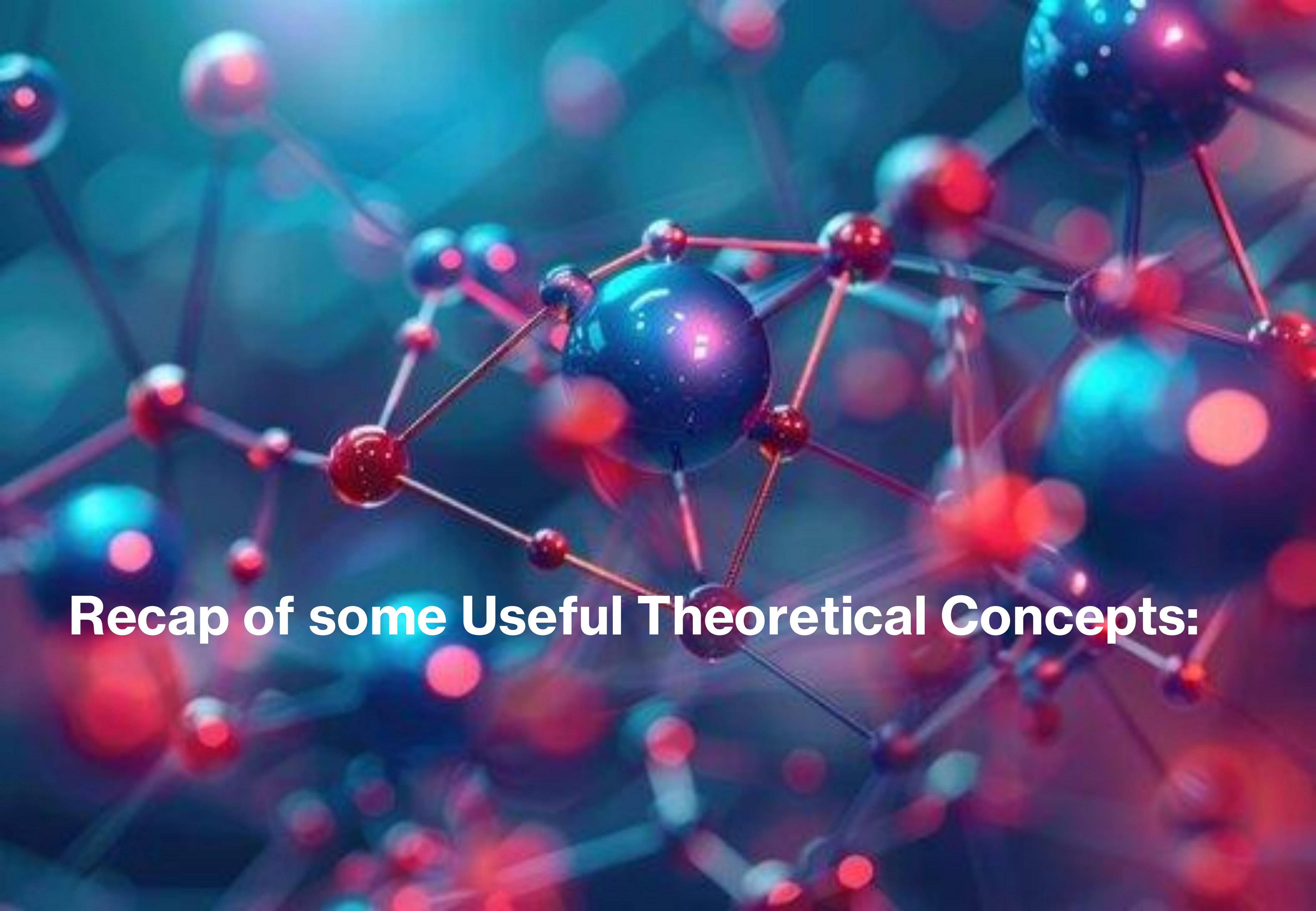
Space-group symmetry	
GENPOS	Generators and General Positions of Space Groups
WYCKPOS	Wyckoff Positions of Space Groups
HKLCOND	Reflection conditions of Space Groups
MAXSUB	Maximal Subgroups of Space Groups
SERIES	Series of Maximal Isomorphic Subgroups of Space Groups
WYCKSETS	Equivalent Sets of Wyckoff Positions
NORMALIZER	Normalizers of Space Groups
KVEC	The k-vector types and Brillouin zones of Space Groups
SYMMETRY OPERATIONS	Geometric interpretation of matrix column representations of symmetry operations
IDENTIFY GROUP	Identification of a Space Group from a set of generators in an arbitrary setting
PROJECTIONS ⚠	Projections of space space groups

Bilbao Crystallographic Server: https://www.cryst.ehu.es/



Recap of some Useful Theoretical Concepts:

Periodic Table of the Elements

1 IA 11A	2 IIA 2A	3 IIIB 3B	4 IVB 4B	5 VB 5B	6 VIB 6B	7 VIIB 7B	8	9 VIII 8	10	11 IB 1B	12 IIB 2B	13 IIIA 3A	14 IVA 4A	15 VA 5A	16 VIA 6A	17 VIIA 7A	18 VIIIA 8A
1 **H** Hydrogen 1.008																	2 **He** Helium 4.003
3 **Li** Lithium 6.941	4 **Be** Beryllium 9.012											5 **B** Boron 10.811	6 **C** Carbon 12.011	7 **N** Nitrogen 14.007	8 **O** Oxygen 15.999	9 **F** Fluorine 18.998	10 **Ne** Neon 20.180
11 **Na** Sodium 22.990	12 **Mg** Magnesium 24.305											13 **Al** Aluminum 26.982	14 **Si** Silicon 28.086	15 **P** Phosphorus 30.974	16 **S** Sulfur 32.066	17 **Cl** Chlorine 35.453	18 **Ar** Argon 39.948
19 **K** Potassium 39.098	20 **Ca** Calcium 40.078	21 **Sc** Scandium 44.956	22 **Ti** Titanium 47.88	23 **V** Vanadium 50.942	24 **Cr** Chromium 51.996	25 **Mn** Manganese 54.938	26 **Fe** Iron 55.933	27 **Co** Cobalt 58.933	28 **Ni** Nickel 58.693	29 **Cu** Copper 63.546	30 **Zn** Zinc 65.39	31 **Ga** Gallium 69.732	32 **Ge** Germanium 72.61	33 **As** Arsenic 74.922	34 **Se** Selenium 78.09	35 **Br** Bromine 79.904	36 **Kr** Krypton 84.80
37 **Rb** Rubidium 84.468	38 **Sr** Strontium 87.62	39 **Y** Yttrium 88.906	40 **Zr** Zirconium 91.224	41 **Nb** Niobium 92.906	42 **Mo** Molybdenum 95.94	43 **Tc** Technetium 98.907	44 **Ru** Ruthenium 101.07	45 **Rh** Rhodium 102.906	46 **Pd** Palladium 106.42	47 **Ag** Silver 107.868	48 **Cd** Cadmium 112.411	49 **In** Indium 114.818	50 **Sn** Tin 118.71	51 **Sb** Antimony 121.760	52 **Te** Tellurium 127.6	53 **I** Iodine 126.904	54 **Xe** Xenon 131.29
55 **Cs** Cesium 132.905	56 **Ba** Barium 137.327	57-71	72 **Hf** Hafnium 178.49	73 **Ta** Tantalum 180.948	74 **W** Tungsten 183.85	75 **Re** Rhenium 186.207	76 **Os** Osmium 190.23	77 **Ir** Iridium 192.22	78 **Pt** Platinum 195.08	79 **Au** Gold 196.967	80 **Hg** Mercury 200.59	81 **Tl** Thallium 204.383	82 **Pb** Lead 207.2	83 **Bi** Bismuth 208.980	84 **Po** Polonium [208.982]	85 **At** Astatine 209.987	86 **Rn** Radon 222.018
87 **Fr** Francium 223.020	88 **Ra** Radium 226.025	89-103	104 **Rf** Rutherfordium [261]	105 **Db** Dubnium [262]	106 **Sg** Seaborgium [266]	107 **Bh** Bohrium [264]	108 **Hs** Hassium [269]	109 **Mt** Meitnerium [268]	110 **Ds** Darmstadtium [269]	111 **Rg** Roentgenium [272]	112 **Cn** Copernicium [277]	113 **Uut** Ununtrium unknown	114 **Fl** Flerovium [289]	115 **Uup** Ununpentium unknown	116 **Lv** Livermorium [298]	117 **Uus** Ununseptium unknown	118 **Uuo** Ununoctium unknown

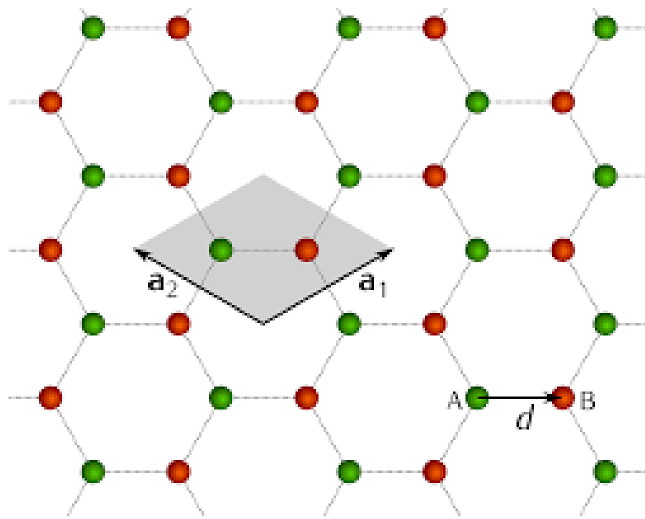
Lanthanide Series	57 **La** Lanthanum 138.906	58 **Ce** Cerium 140.115	59 **Pr** Praseodymium 140.908	60 **Nd** Neodymium 144.24	61 **Pm** Promethium 144.913	62 **Sm** Samarium 150.36	63 **Eu** Europium 151.966	64 **Gd** Gadolinium 157.25	65 **Tb** Terbium 158.925	66 **Dy** Dysprosium 162.50	67 **Ho** Holmium 164.930	68 **Er** Erbium 167.26	69 **Tm** Thulium 168.934	70 **Yb** Ytterbium 173.04	71 **Lu** Lutetium 174.967
Actinide Series	89 **Ac** Actinium 227.028	90 **Th** Thorium 232.038	91 **Pa** Protactinium 231.036	92 **U** Uranium 238.029	93 **Np** Neptunium 237.048	94 **Pu** Plutonium 244.064	95 **Am** Americium 243.061	96 **Cm** Curium 247.070	97 **Bk** Berkelium 247.070	98 **Cf** Californium 251.080	99 **Es** Einsteinium [254]	100 **Fm** Fermium 257.095	101 **Md** Mendelevium 258.1	102 **No** Nobelium 259.101	103 **Lr** Lawrencium [262]

Alkali Metal	Alkaline Earth	Transition Metal	Semimetal	Nonmetal	Basic Metal	Halogen	Noble Gas	Lanthanide	Actinide

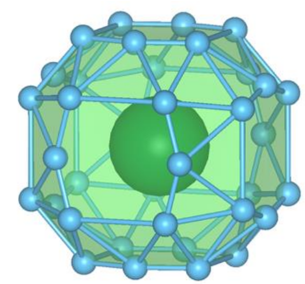
Crystal Lattices:

A crystal lattice is generated by periodically repeating the same **unit cell**, defined by 3 ***lattice* vectors** and **m *basis*** vectors:

$$\mathbf{R}_i = \mathbf{R} + \boldsymbol{\tau}_i, \qquad \mathbf{R} = n_1\mathbf{R}_1 + n_2\mathbf{R}_2 + n_3\mathbf{R}_3$$
$$i = 1, \ldots, m$$



In addition to **Translational Symmetry** (Bloch's theorem) many crystals exhibit additional symmetry operations, giving rise to highly complex (and beautiful) structures.



Symmetry Operations in Crystals:

Definition: A **symmetry operation** is a transformation that maps a crystal structure onto itself, preserving the arrangement and orientation of atoms within the lattice.

Types of Symmetry Operations (3D):

- **Translation**
- **Identity**
- **Inversion**
- ***n*-Fold Rotation (**Rotation by 360/n**).**
- ***Mirror Plane* Reflection**
- **n-Fold Rotoinversion (**Rotation by 360/n **+ Inversion)**
- **Glide Planes**
- **Screw Axes**

Depending on their symmetry properties, all known crystal structures can be classified into **230** distinct **space groups (3D).**

Space Groups (1):

The **230 Space Groups** are obtained combining the symmetry properties of the underlying **Bravais Lattice** (Translations) with local symmetries defined by the **point group**.

Crystallographic Point Groups: A **point group** is a mathematical set of symmetry operations, such as rotations, reflections, and inversions, that leave at least one point fixed and characterize the local symmetry around that point. Point groups are used to describe the symmetry of finite objects (molecules, small portions of a crystal).

There is in principle an infinite number of possible symmetry operations and hence point groups; however, in a 3D crystal, the necessity to tessellate space reduces the number and type of symmetry operations, leading **to 32 crystallographic point groups.**

Bravais Lattices: A **Bravais lattice** is a set of discrete points in space generated by applying all integer linear combinations of three non-coplanar basis vectors $\mathbf{R}_1$, $\mathbf{R}_2$, $\mathbf{R}_3$:

$$\mathbf{R} = n_1\mathbf{R}_1 + n_2\mathbf{R}_2 + n_3\mathbf{R}_3$$

A Bravais Lattice is invariant under a lattice vector translation. In three dimensions, there are **14 unique Bravais lattices**.

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Space Groups (2):

The **230 Space Groups** are obtained combining the symmetry properties of the underlying **Bravais Lattice** (Translations) with local symmetries defined by the **point group**.

Types of Symmetry Operations:

- **Translation**
- **Identity**
- **Inversion**
- ***n*-Fold Rotation *(2,3,4,6)***
- ***Mirror Plane* Reflection**
- **n-Fold Rotoinversion *(2,3,4,6)***
- **Glide Planes**
- **Screw Axes**

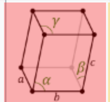
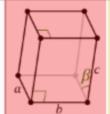
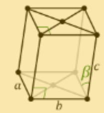
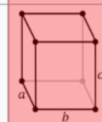
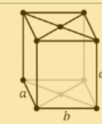
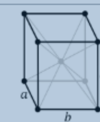
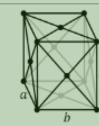
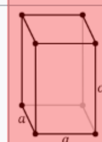
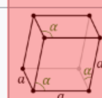
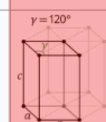
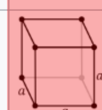
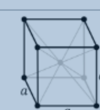
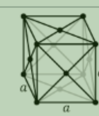
Crystallographic
Point Group Operations

Mirror + Translation

Rotation + Translation

Bravais Lattices in 3d (14)

P=primitive I=Innenzentriert F=Flaechenzentriert

Crystal family	Lattice system	Point group (Schönflies notation)	14 Bravais lattices			
			Primitive (P)	Base-centered (S)	Body-centered (I)	Face-centered (F)
Triclinic (a)		C_i	 aP			
Monoclinic (m)		C_{2h}	 mP	 mS		
Orthorhombic (o)		D_{2h}	 oP	 oS	 oI	 oF
Tetragonal (t)		D_{4h}	 tP		 tI	
Hexagonal (h)	Rhombohedral	D_{3d}	 hR			
	Hexagonal	D_{6h}	 hP			
Cubic (c)		O_h	 cP		 cI	 cF

a,b,c base-centered

Crystallographic Point Groups (32)

1. Cubic System (5 point groups)
   - $m\bar{3}m$ (O_h): **Includes 3 four-fold, 4 three-fold, and 6 two-fold rotations, plus inversion and mirror planes.**
   - **432** (O): **3 four-fold rotations and 4 three-fold rotations, without inversion.**
   - $m\bar{3}$ (T_h): **Inversion with 4 three-fold rotations and mirror planes.**
   - **23** (T): **3 two-fold and 4 three-fold rotations.**
   - $\bar{4}3m$ (T_d): **4 three-fold rotations and mirror planes (without inversion).**
2. Tetragonal System (7 point groups)
   - **4/mmm** (D_{4h}): **Four-fold rotation, inversion, and mirror planes.**
   - **4/m** (S_4): **Four-fold rotation with inversion.**
   - **422** (D_4): **Four-fold rotation and two-fold rotations, no inversion.**
   - **4mm** (C_{4v}): **Four-fold rotation and mirror planes.**
   - **4** (C_4): **Four-fold rotation only.**
   - $\bar{4}2m$ (S_4): **Rotoinversion with mirror planes.**
   - $\bar{4}$ (C_{4h}): **Four-fold rotoinversion.**
3. Hexagonal System (7 point groups)
   - **6/mmm** (D_{6h}): **Six-fold rotation, mirror planes, and inversion.**
   - **6/m** (C_{6h}): **Six-fold rotation with inversion.**
   - **622** (D_6): **Six-fold and two-fold rotations.**
   - **6mm** (C_{6v}): **Six-fold rotation with mirror planes.**
   - **6** (C_6): **Six-fold rotation only.**
   - $\bar{6}m2$ (D_{3h}): **Six-fold rotoinversion with mirror planes.**
   - $\bar{6}$ (C_{3h}): **Six-fold rotoinversion.**
4. Trigonal (Rhombohedral) System (5 point groups)
   - **3m** (C_{3v}): **Three-fold rotation with mirror planes.**
   - **3** (C_3): **Three-fold rotation only.**
   - **32** (D_3): **Three-fold rotation and two-fold rotations.**
   - $\bar{3}$ (C_{3i}): **Three-fold rotoinversion.**
   - $\bar{3}m$ (D_{3d}): **Three-fold rotoinversion with mirror planes.**
5. Orthorhombic System (3 point groups)
   - **mmm** (D_{2h}): **Two-fold rotations along three perpendicular axes, inversion, and mirror planes.**
   - **222** (D_2): **Two-fold rotations along three perpendicular axes, no inversion.**
   - **mm2** (C_{2v}): **Two-fold rotation with mirror planes.**
6. Monoclinic System (2 point groups)
   - **2/m** (C_{2h}): **Two-fold rotation with inversion and a mirror plane.**
   - **2** (C_2): **Two-fold rotation only.**
7. Triclinic System (1 point group)
   - $\bar{1}$ (C_i): **Inversion only.**

Space Groups:

The 230 Space Groups are obtained combining the symmetry properties of the underlying Bravais Lattices (Translations) with local symmetries defined by the point group.

List of Space Groups (230):

Bravais Lattice	Space Group	
Triclinic (P)	1–2	**2**
Monoclinic (P,C)	3–15	**13**
Orthorhombic (P,C,I,F)	16–74	**59**
Tetragonal (P,I)	75–142	**68**
Trigonal (P,R)	143–167	**25**
Hexagonal (P)	168–194	**27**
Cubic (P,I,F)	195–230	**36**

Wyckoff Positions

Wyckoff positions describe the specific **coordinates** in the unit cell where atoms can be placed, respecting the symmetry of the space group. Each Wyckoff position has an associated **multiplicity** (how many symmetry-equivalent positions exist) and **site symmetry** (the symmetry elements at that position).

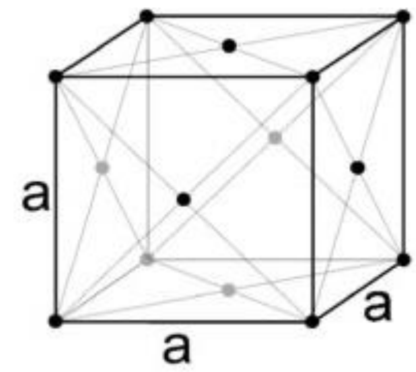
Each Wyckoff position is represented by:
1. A **multiplicity**: The number of symmetry-equivalent positions in the unit cell.
2. A **letter**: Alphabetically ordered starting from **a**, with **a** representing the site with highest symmetry.
3. **Coordinates**: The specific fractional coordinates (x, y, z) of the position in the unit cell.
4. **Site symmetry**: The symmetry present at the specific Wyckoff position (e.g., m3m, 4mm), which is a subgroup of the overall space group symmetry.

Fm-3m (225) space group

8	c	-43m	(1/4,1/4,1/4) (1/4,1/4,3/4)
4	b	m-3m	(1/2,1/2,1/2)
4	a	m-3m	(0,0,0)

https://www.cryst.ehu.es/cgibin/cryst/programs/nph-wp-list

Example: The Fm-3m (225) space group



Face-centered cubic (F)

The **Fm-3m** space group has **48** symmetry operations:

Identity (1)

Inversion (1)

Rotations (23):

- **3-fold (120,240) rotations** around one of the **4 body diagonals: 8**
- **4-fold (90) rotations** around one of the **6 cube edges: 6**
- **2-fold rotations** about the **midpoint** of the **edges (6) +** through **face centers (3): 9**

Mirror Planes (9):

- Parallel to **Cube Faces (3)**
- Parallel to **Face Diagonals (6)**

Glide Planes (6):

- **Reflection** along one of the *(xy), (xz), (yz)* planes in (0,0,0) or midpoint (x/2), (y/2) or (z/2) + ½ **translation** (**a,b,c**) glide planes.

Screw Axes (8):

- **Two-fold rotation** along (100), (010), (001) or (111) directions + ½ translation **(4)**
- **Three-fold rotations** along (111), (-111), (1-11), (11-1) + 1/3 or 2/3 translation **(4)**

In matrix notation:

$$\mathbf{r}' = M\mathbf{r} + \mathbf{t}$$

Identity:

$$M = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \mathbf{t} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

90 rotation along z (4-fold):

$$M = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \mathbf{t} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

180 (2-fold) screw: 180 Rotation around x + ½ translation:

$$M = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad \mathbf{t} = \begin{pmatrix} \frac{1}{2} \\ 0 \\ 0 \end{pmatrix}$$

Space Group Tables

Wyckoff positions (Fm-3m space group):

Multiplicity	Wyckoff letter	Site symmetry	Coordinates
			(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) +
192	l	1	(x,y,z) (-x,-y,z) (-x,y,-z) (x,-y,-z) (z,x,y) (z,-x,-y) (-z,-x,y) (-z,x,-y) (y,z,x) (-y,z,-x) (y,-z,-x) (-y,-z,x) (y,x,-z) (-y,-x,-z) (y,-x,z) (-y,x,z) (x,z,-y) (-x,z,y) (-x,-z,-y) (x,-z,y) (z,y,-x) (z,-y,x) (-z,y,x) (-z,-y,-x) (-x,-y,-z) (x,y,-z) (x,-y,z) (-x,y,z) (-z,-x,-y) (-z,x,y) (z,x,-y) (z,-x,y) (-y,-z,-x) (y,-z,x) (-y,z,x) (y,z,-x) (-y,-x,z) (y,x,z) (-y,x,-z) (y,-x,-z) (-x,-z,y) (x,-z,-y) (x,z,y) (-x,z,-y) (-z,-y,x) (-z,y,-x) (z,-y,-x) (z,y,x)
96	k	..m	(x,x,z) (-x,-x,z) (-x,x,-z) (x,-x,-z) (z,x,x) (z,-x,-x) (-z,-x,x) (-z,x,-x) (x,z,x) (-x,z,-x) (x,-z,-x) (-x,-z,x) (x,x,-z) (-x,-x,-z) (x,-x,z) (-x,x,z) (x,z,-x) (-x,z,x) (-x,-z,-x) (x,-z,x) (z,x,-x) (z,-x,x) (-z,x,x) (-z,-x,-x)
96	j	m..	(0,y,z) (0,-y,z) (0,y,-z) (0,-y,-z) (z,0,y) (z,0,-y) (-z,0,y) (-z,0,-y) (y,z,0) (-y,z,0) (y,-z,0) (-y,-z,0) (y,0,-z) (-y,0,-z) (y,0,z) (-y,0,z) (0,z,-y) (0,z,y) (0,-z,-y) (0,-z,y) (z,y,0) (z,-y,0) (-z,y,0) (-z,-y,0)
48	i	m.m 2	(1/2,y,y) (1/2,-y,y) (1/2,y,-y) (1/2,-y,-y) (y,1/2,y) (y,1/2,-y) (-y,1/2,y) (-y,1/2,-y) (y,y,1/2) (-y,y,1/2) (y,-y,1/2) (-y,-y,1/2)
48	h	m.m 2	(0,y,y) (0,-y,y) (0,y,-y) (0,-y,-y) (y,0,y) (y,0,-y) (-y,0,y) (-y,0,-y) (y,y,0) (-y,y,0) (y,-y,0) (-y,-y,0)
48	g	2.m m	(x,1/4,1/4) (-x,3/4,1/4) (1/4,x,1/4) (1/4,-x,3/4) (1/4,1/4,x) (3/4,1/4,-x) (1/4,x,3/4) (3/4,-x,3/4) (x,1/4,3/4) (-x,1/4,1/4) (1/4,1/4,-x) (1/4,3/4,x)
32	f	.3m	(x,x,x) (-x,-x,x) (-x,x,-x) (x,-x,-x) (x,x,-x) (-x,-x,-x) (x,-x,x) (-x,x,x)
24	e	4m. m	(x,0,0) (-x,0,0) (0,x,0) (0,-x,0) (0,0,x) (0,0,-x)
24	d	m.m m	(0,1/4,1/4) (0,3/4,1/4) (1/4,0,1/4) (1/4,0,3/4) (1/4,1/4,0) (3/4,1/4,0)
8	c	-43m	(1/4,1/4,1/4) (1/4,1/4,3/4)
4	b	m-3m	(1/2,1/2,1/2)
4	a	m-3m	(0,0,0)

Site-symmetry point group

4a and 4b sites retain the full symmetry of the lattice, other Wyckoff positions have a lower symmetry (point group). Site symmetry/point group - https://www.cryst.ehu.es/cgi-bin/cryst/programs/nph-wp-list.

Symmetry operations (m-3m point group):

Identity (1)

Inversion (1)

Rotations (23):

- **3-fold (120,240) rotations** around one of the **4 body diagonals: 8**
- **4-fold (90) rotations** around one of the **6 cube edges: 6**
- **2-fold rotations** about the **midpoint** of the **edges (6) +** through **face centers (3): 9**

Mirror Planes (9):

- Parallel to **Cube Faces (3)**
- Parallel to **Face Diagonals (6)**

4-fold rotoinversions (6):

- **Rotation** around the cube edges, followed by inversion.

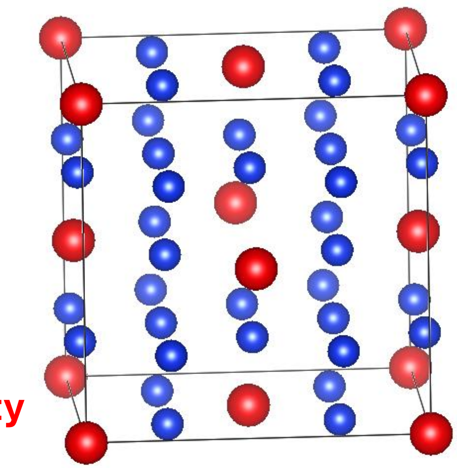
3-fold rotoinversions (8):

- **Three-fold rotations** along (111), (-111), (1-11), (11-1) followed by inversion **(8)**

Site Symmetry space groups:

Site symmetry point groups have equal or lower symmetry than the full symmetry space group of the crystal:

Example, position 24d, has 8 site symmetry operations (mmm):



Space Group : *Fm-3m* (No. 225)
Point : (0,1/4,1/4)
Wyckoff Position : 24d

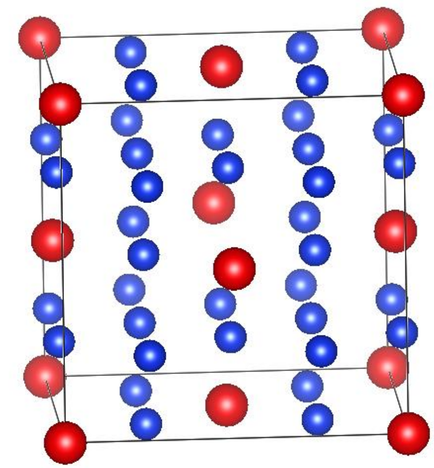
Site Symmetry Group m.m m

x,y,z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	1	Identity
-x,z,y	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$	2 0,y,y	2-fold rotation
-x,y,z	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	m 0,y,z	Mirror
x,z,y	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$	m x,y,y	Mirror
x,-y+1/2,-z+1/2	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1/2 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}$	2 x,1/4,1/4	2-fold Rotation
-x,-z+1/2,-y+1/2	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 1/2 \\ 0 & -1 & 0 & 1/2 \end{pmatrix}$	2 0,y+1/2,-y	2-fold Rotation
-x,-y+1/2,-z+1/2	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1/2 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}$	-1 0,1/4,1/4	Inversion
x,-z+1/2,-y+1/2	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 1/2 \\ 0 & -1 & 0 & 1/2 \end{pmatrix}$	m x,y+1/2,-y	Mirror

Space Group Tables

Site symmetry point groups have equal or lower symmetry than the full symmetry space group of the crystal:

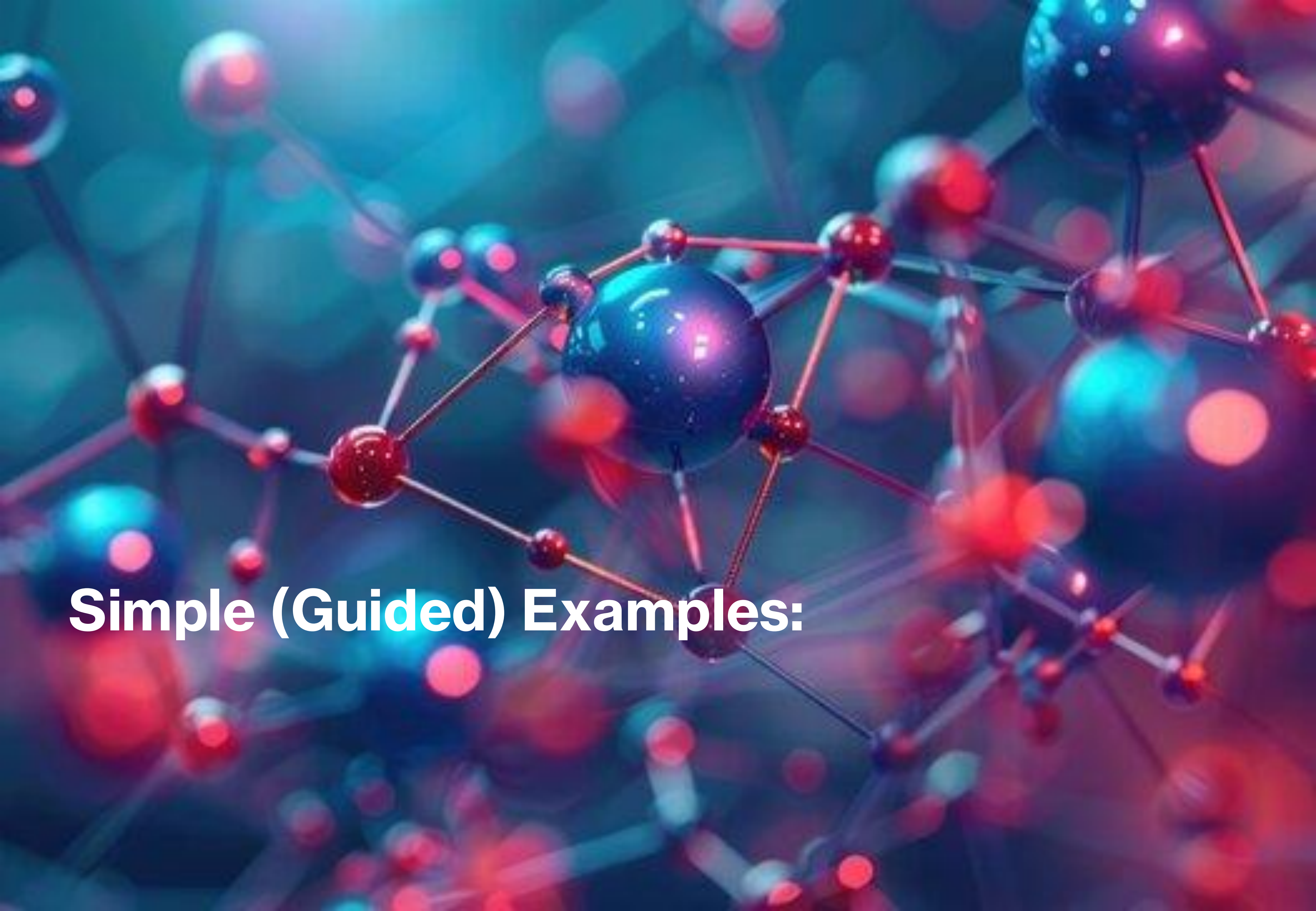
Example, position 24d, has 8 site symmetry operations (mmm):



5. Orthorhombic System (3 point groups)

- **mmm (D_{2h}): Two-fold rotations along three perpendicular axes, inversion, and mirror planes.**
- **222 (D_2): Two-fold rotations along three perpendicular axes, no inversion.**
- **mm2 (C_{2v}): Two-fold rotation with mirror planes.**

Simple (Guided) Examples:



Silicon (Diamond) Structure

Crystal Structure

Lattice (Primitive)

a	3.85 Å
b	3.85 Å
c	3.85 Å
α	60.00 °
β	60.00 °
γ	60.00 °
Volume	40.33 Å^3

Lattice is given in its primitive crystallographic setting.

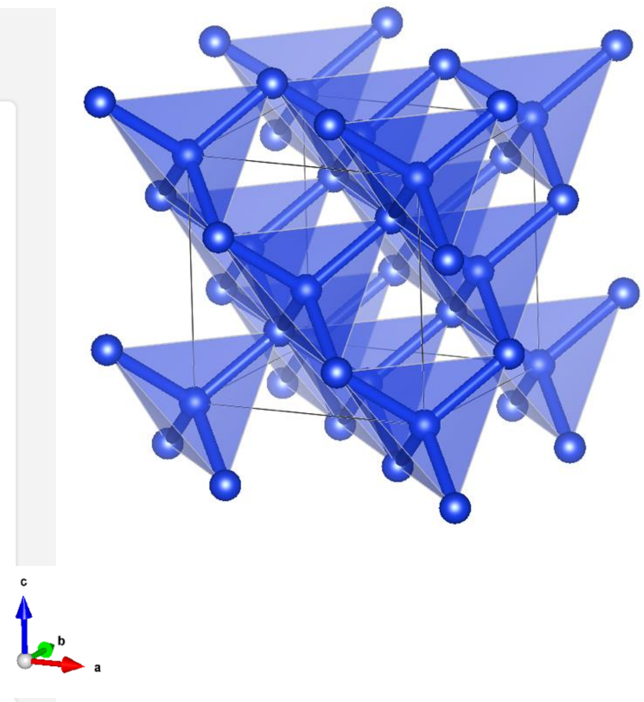
Atomic Positions

Wyckoff	Element	x	y	z
8a	Si	3/4	3/4	1/4

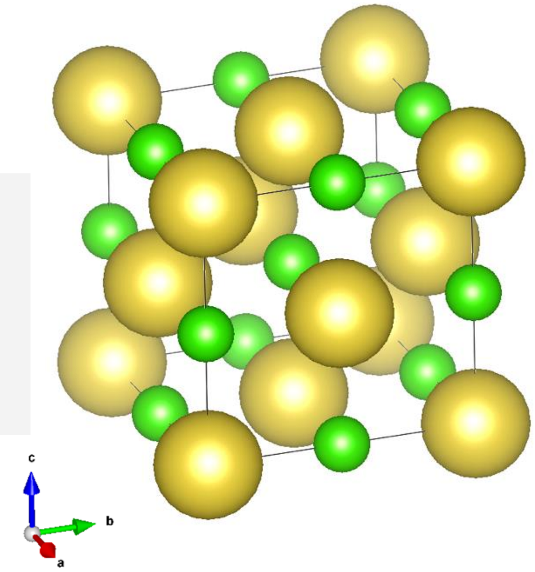
Symmetry

Crystal System	Cubic
Lattice System	Cubic
Hall Number	F 4d 2 3 -1d
International Number	227 fcc
Symbol	Fd$\bar{3}$m
Point Group	m$\bar{3}$m

Number of Atoms	8
Density	2.31 g·cm^{-3}
Dimensionality	3D
Possible Oxidation States	Unknown



NaCl (Rocksalt) Structure



Crystal Structure

Lattice (Primitive)

a	3.95 Å
b	3.95 Å
c	3.95 Å
α	60.00 °
β	60.00 °
γ	60.00 °
Volume	43.63 Å^3

Lattice is given in its primitive crystallographic setting.

Atomic Positions

Wyckoff	Element	x	y	z
4a	Na	0	0	0
4b	Cl	0	0	1/2

Symmetry

Crystal System	Cubic
Lattice System	Cubic
Hall Number	-F 4 2 3
International Number	225 **fcc**
Symbol	Fm$\bar{3}$m
Point Group	m$\bar{3}$m

Number of Atoms	8
Density	2.22 g·cm^{-3}
Dimensionality	3D
Possible Oxidation States	Cl^-, Na^+

TODO: Exercise

Superconductivity in sodalite-like yttrium hydride clathrates

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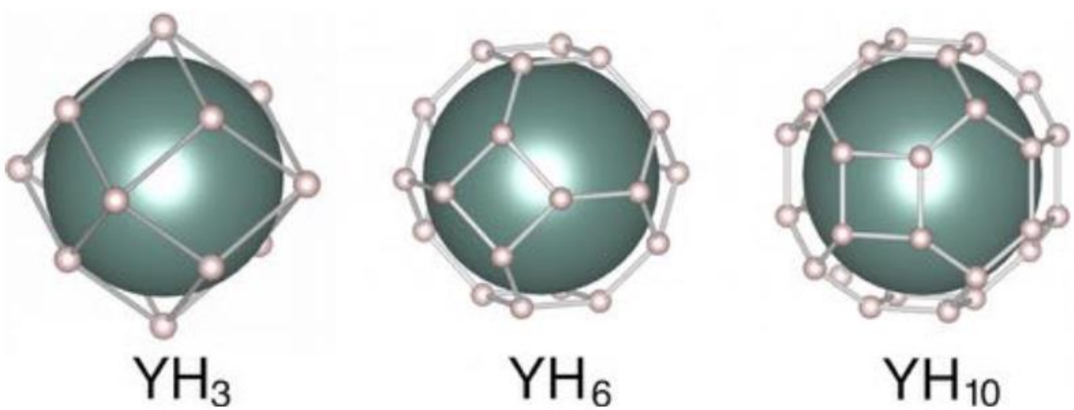
Table S1. Structural data for YH_3, YH_6 and YH_{10} at 300 GPa.

	spc. gr.	a (Å)	Y	H_1	H_2
YH_3	225	4.007	$4b$ (1/2, 1/2, 1/2)	$4a$ (0, 0, 0)	$8c$ (1/4, 1/4, 1/4)
YH_6	229	3.369	$2a$ (0,0,0)	$12d$ (0,1/2,1/4)	-
YH_{10}	225	4.600	$4a$ ~~(1/2,1/2,1/2)~~ (0,0,0)	$8c$ ~~(0,0,0)~~ (1/4,1/4,1/4)	$32f$ (x,x,x) x=0.380

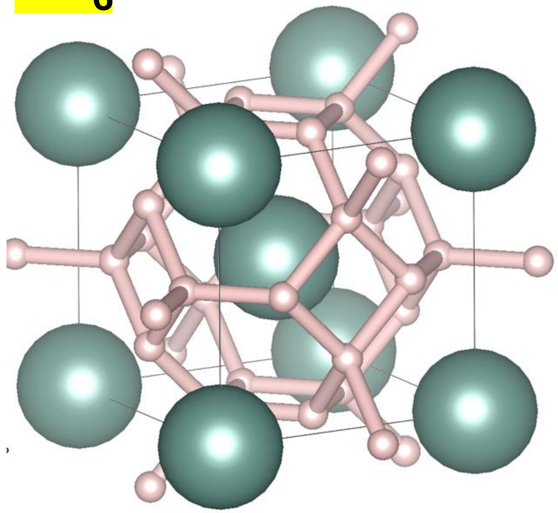


Yttrium sodalite-clathrate Hydrides:

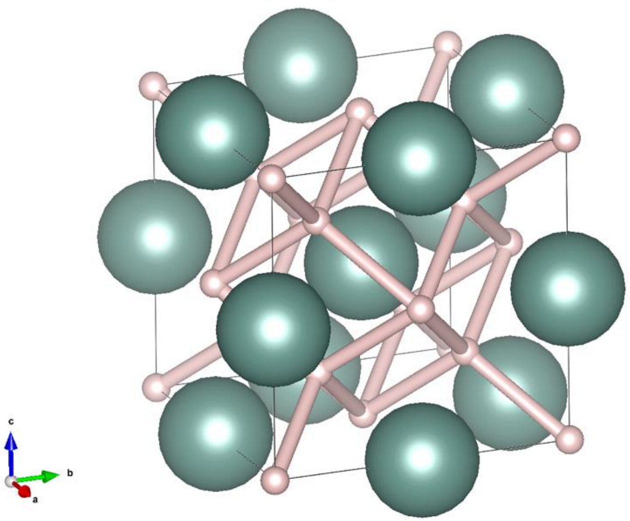
Consider the three structures in the previous slide. They represent three different types of Yttrium Hydrides, which form at extreme pressures (>200 GPa).
Using the information in the previous tables, set up the three crystal structures and answer the following questions:

- What is the space group of the structure?
- What type of Bravais lattice does it correspond to?
- How many inequivalent atoms are there? What are their Wyckoff Positions?
- What is the multiplicity of the Wyckoff positions? Are they fixed or free?
- What is the corresponding point group? How many symmetry operation does the point group have?
- What is the shortest Y-H and H-H distance?
- Which structure has the smallest volume?
- Which one has the shortest H-H distance?
- What is the **density** of **H atoms** in the structure?

YH_6



YH_3



YH_{10}