Survey of Materials. Lecture 2

Atomistic structure

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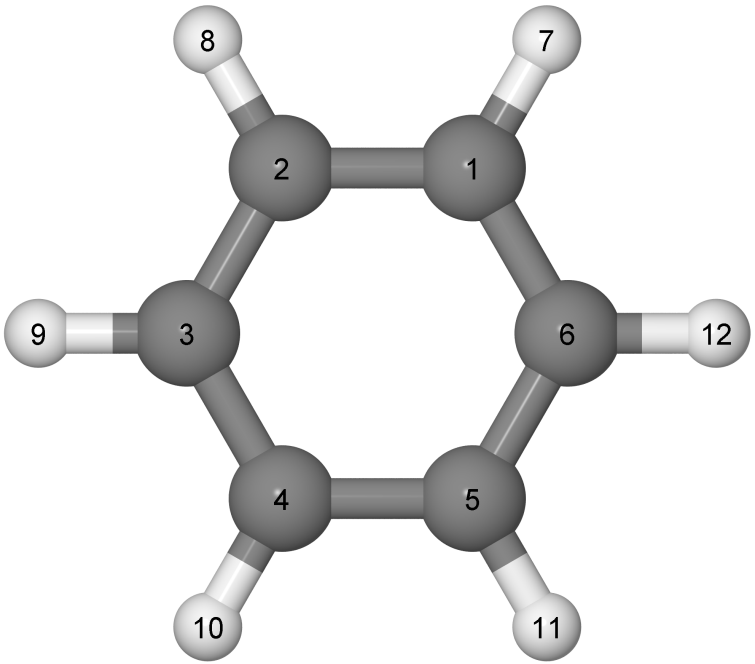
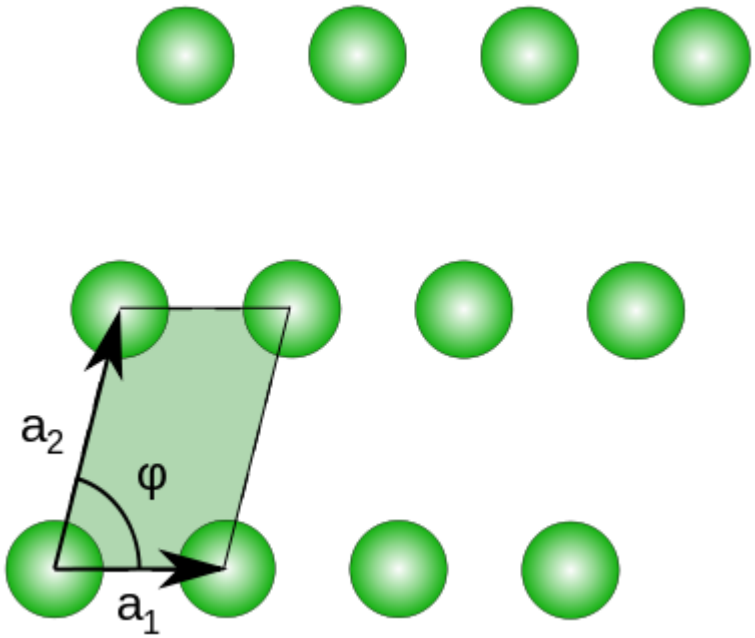
Outline

- Why symmetry is important
- 2D crystallography
- 3D crystallography
- Nonperiodic solids
- Structure characterization and determination

2D crystallography

Space group = point group + translation symmetry

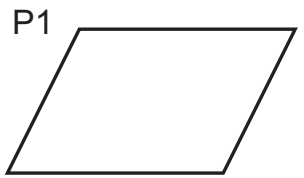


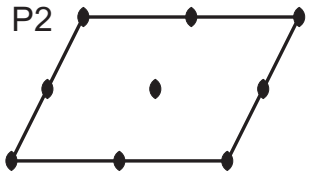


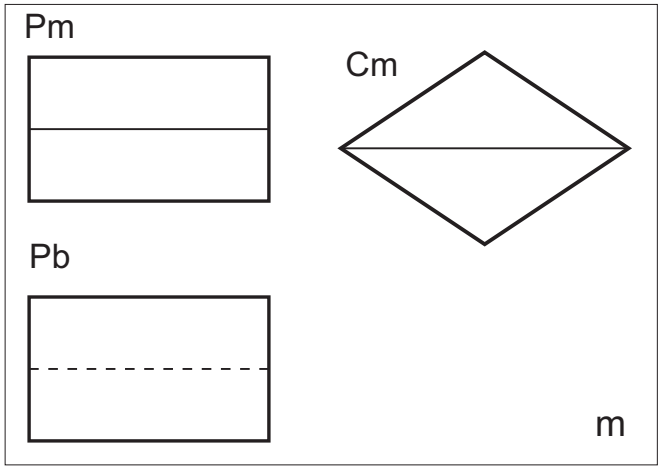
- Determine all 2D point groups
- Determine all 2D Bravais lattices

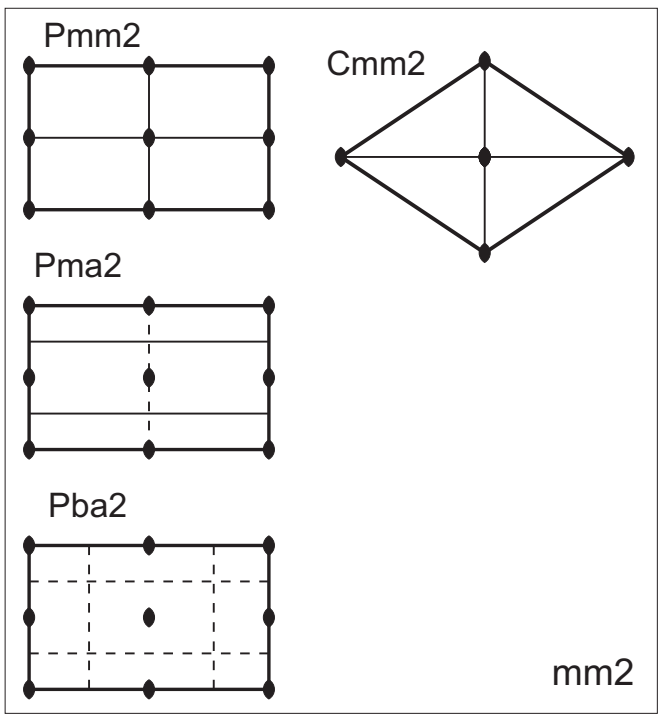
2D crystallography

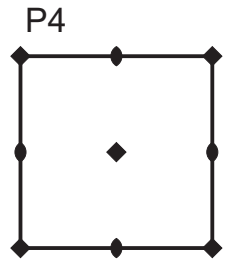
2D space groups (17), point groups, Bravais lattices, and crystal systems (4)

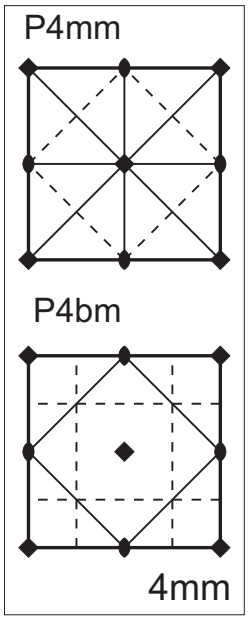


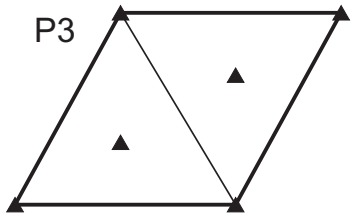


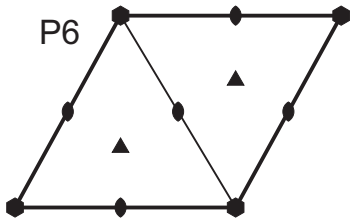


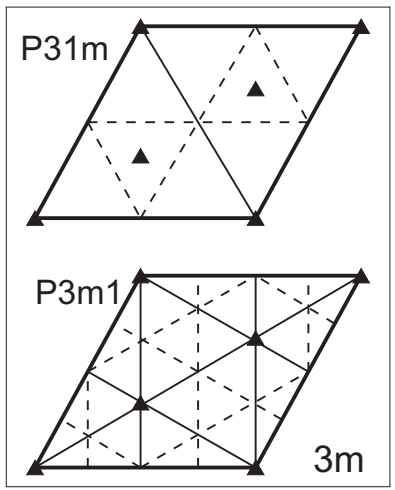


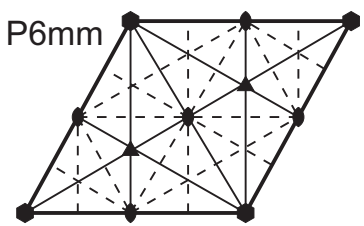












Bravais lattices:

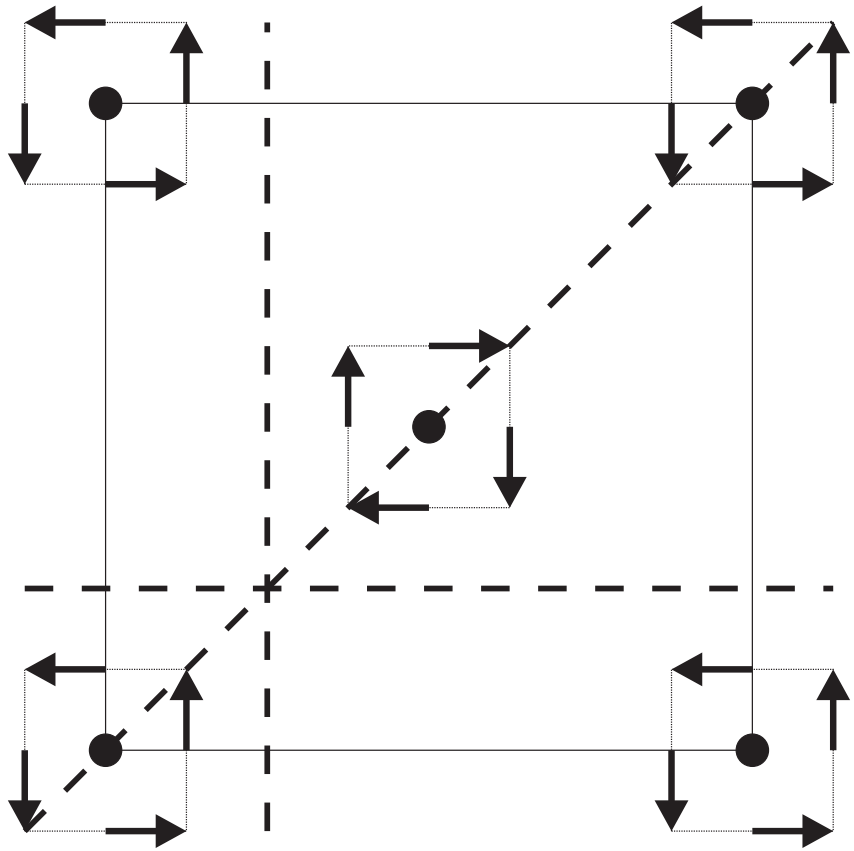
P2	oblique
Pmm2	rectangular
Cmm2	rhombic
P4mm	square
P6mm	hexagonal

Point groups:

1-6	$C_{1\text{-}6}$
m	D_1
mm2	D_2
3m	D_3
4mm	D_4
6mm	D_6

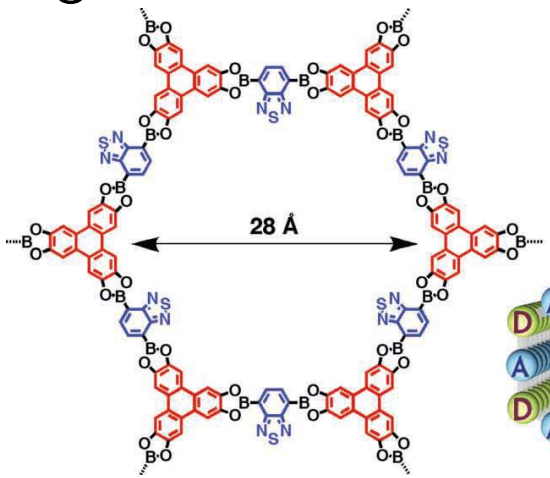
Symmetries:

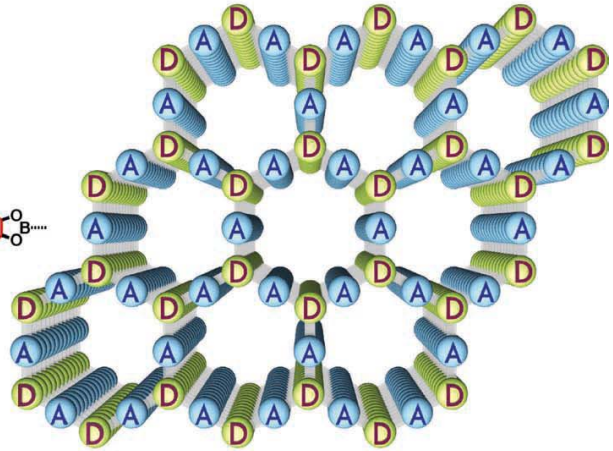
2D glide plane



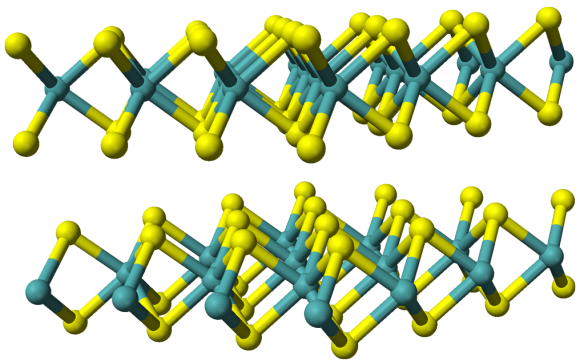
2D materials

- graphene, BN
- organic networks



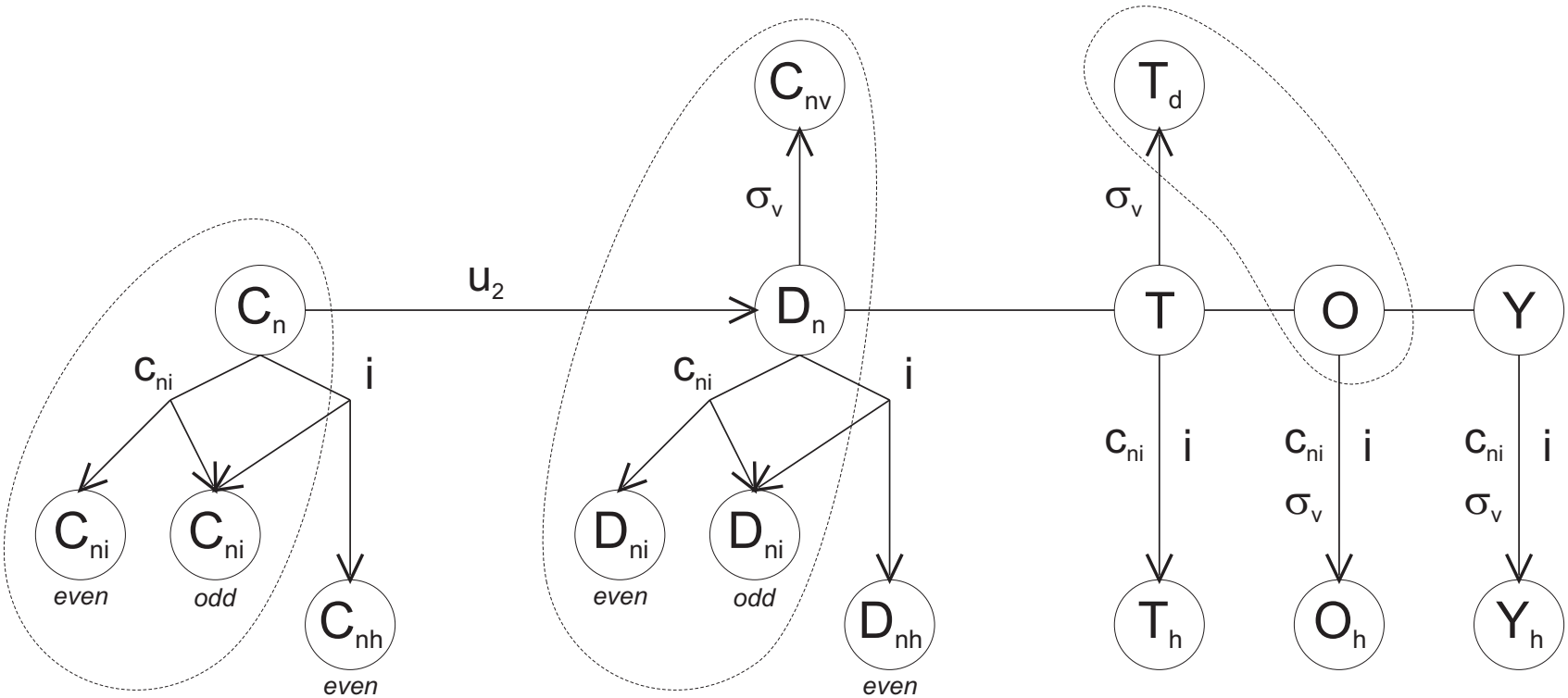


- MoS_2

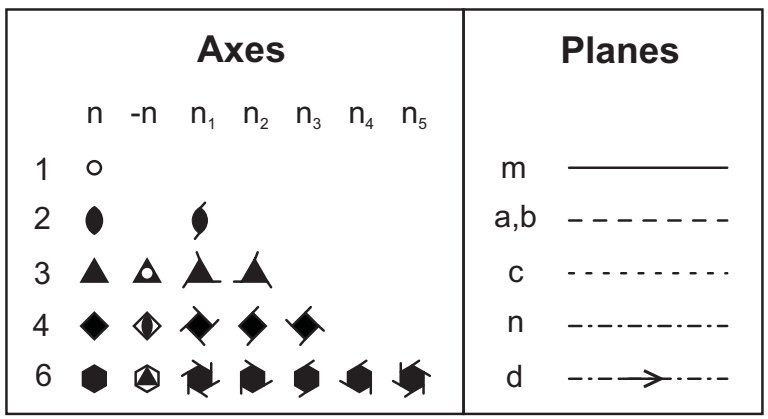


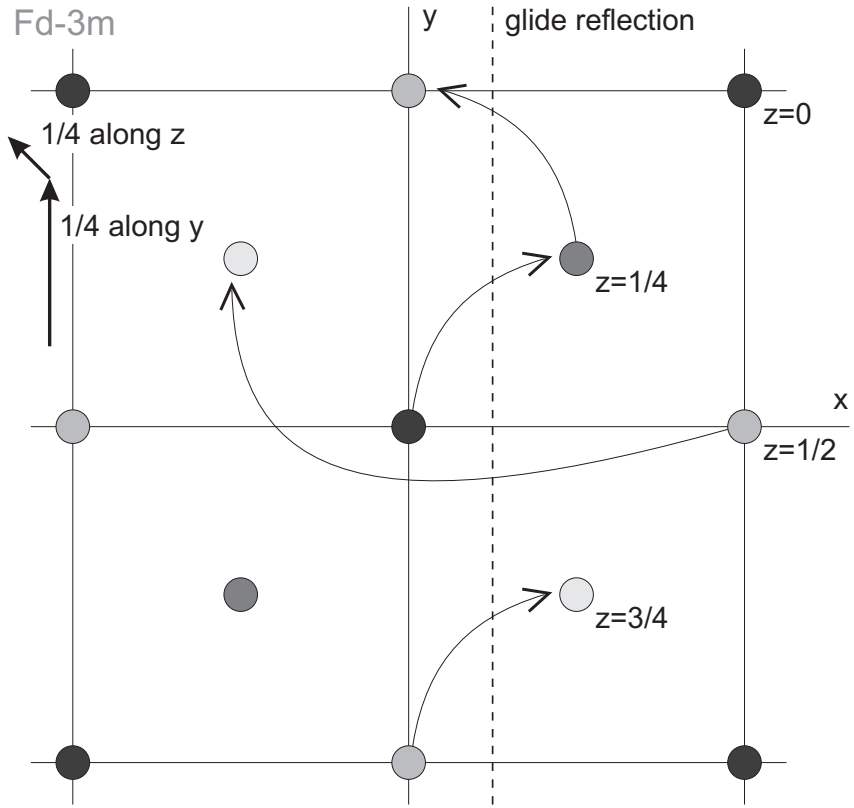
- P, As

3D point groups



3D symmetry elements

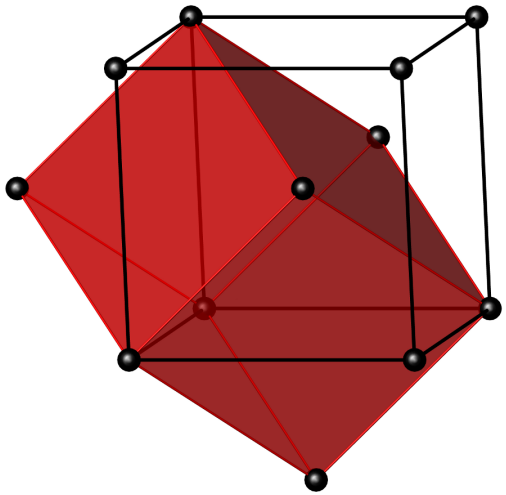


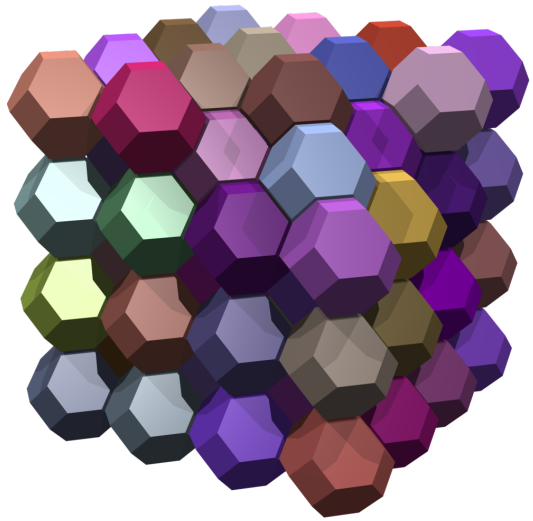


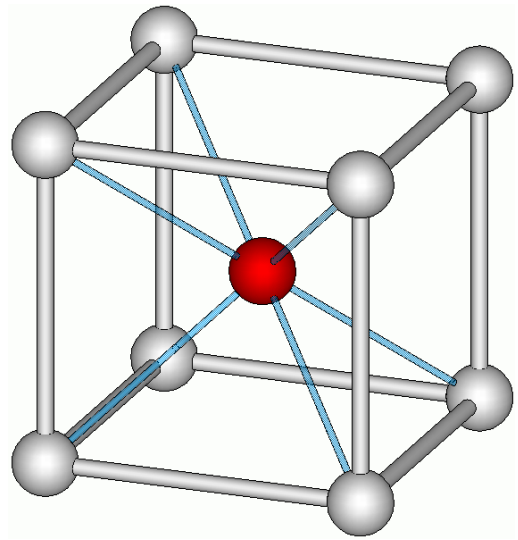
3D crystallography

Lecture of Artem Abakumov or any textbook

Unit cell







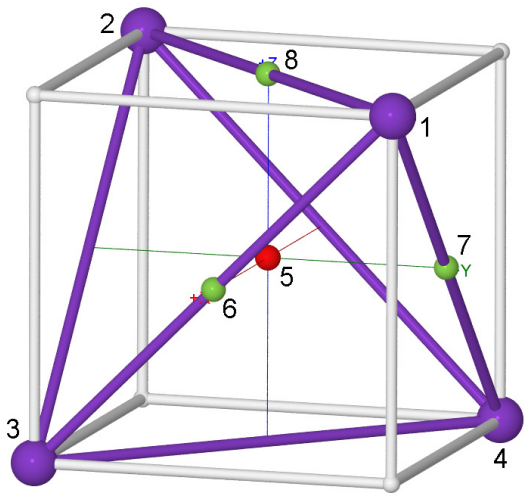
	min.size	parallelepiped	symmetric
primitive	+	+	−
Wigner–Seitz	+	−	+
Bravais	−	+	+

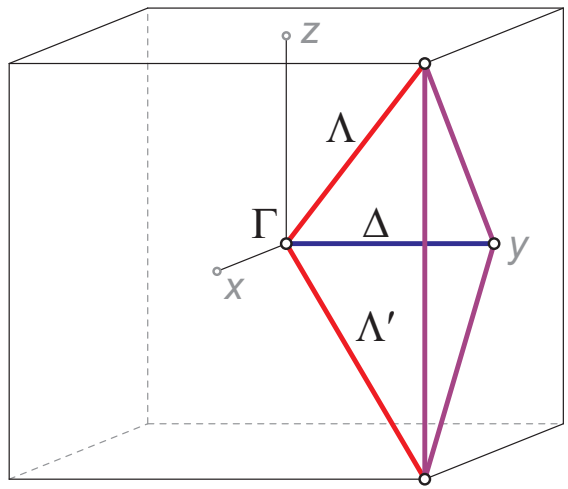
Generators, fundamental domain, asymmetric unit

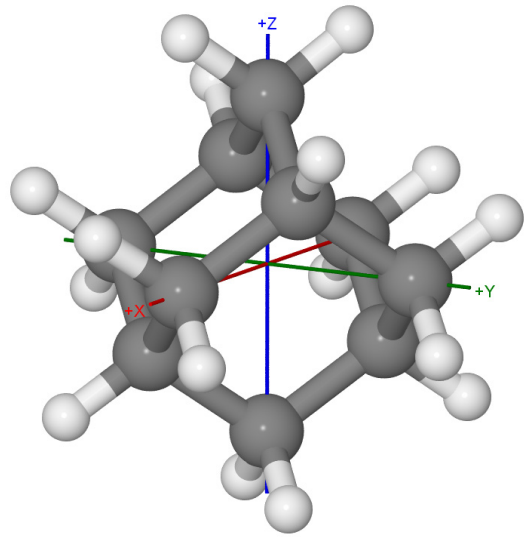
also orbits (Wyckoff positions), stabilizators, independent geometrical parameters etc.

-43m $\equiv T_d = \{1, 8c_3, 3c_2, 6c_{4i}, 6\sigma_v\} \sim O$

Generators: $c_3(1)$ and $\sigma_v(34)$, e.g. $c_3(1)\sigma_v(34) = c_{4i}^{-1}(7)$, $c_{4i}^2 = c_2$







	orbit	WP	stab.	atoms
000	Γ	1a	-43m	
xxx	Λ	4e	3m	CH
x00	Δ	6f	2mm	C
xxz	ΛΔ	12i	m	H
xyz		24j	1	

Fundamental domain is $\Lambda\Delta\Lambda'$-pyramid ($V = 1/24$)

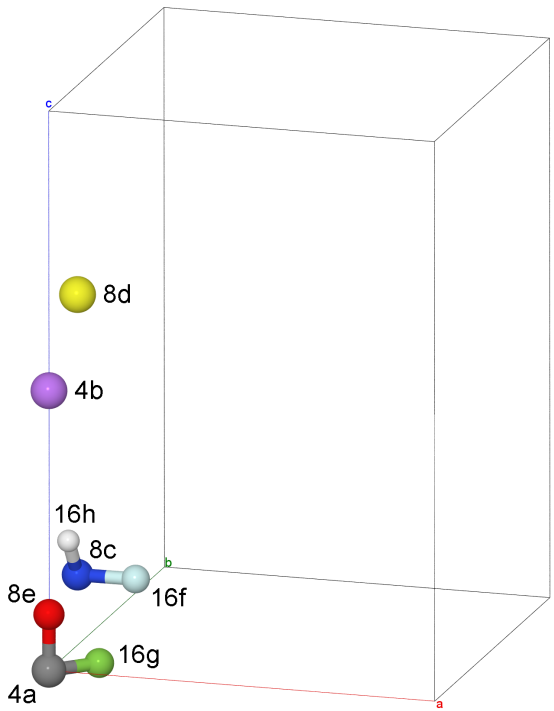
Asymetric unit is HCCH

Geometrical parameters are CC, 2×CH, CCC, HCH or $x(C_1), x(H_1), x(C_2), x(H_2), z(H_2)$

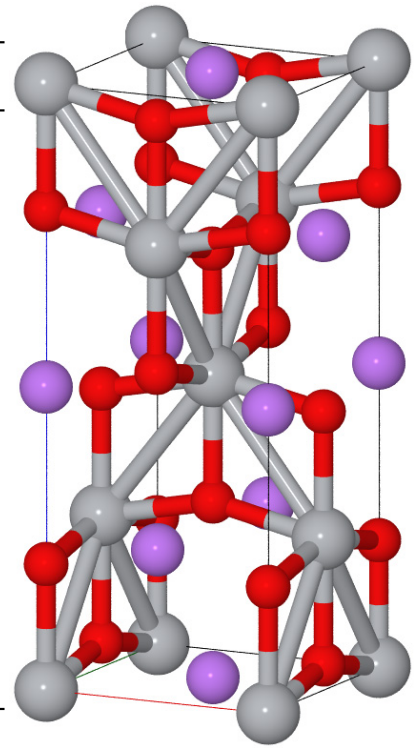
The same for crystal

I41/amd:1 $\equiv D_{4h}^{19}$

Generators: -4_{001}, 2_{110}, $\left(\frac{1}{2}\frac{1}{2}\frac{1}{2}\right)$, $\left\{-1\left|0\frac{1}{2}\frac{1}{4}\right.\right\}$, (100), (010), (001)



	WP	stab.	atom
000	4a	-4m2	Ti
$00\frac{1}{2}$	4b	-4m2	Li
$0\frac{1}{4}\frac{1}{8}$	8c	.2/m.	
$0\frac{1}{4}\frac{5}{8}$	8d	.2/m.	
$00z$	8e	2mm.	O
$x\frac{1}{4}\frac{1}{8}$	16f	.2.	
$xx0$	16g	..2	
$0yz$	16h	.m.	
xyz	32i	1	



Fundamental domain is the box $(1/2, 1/2, 1/8)$ with $V = 1/32$

Asymetric unit is TiOLi

Geometrical parameters are a, c, ζ or 2×TiO and OTiO

Classification of space groups

structural type	A4 (dia)	A3 (hcp)	A7 (α-As)
space group	Fd-3m	P63/mmc	R-3m
arithmetic crystal class	Fm-3m	P6/mmm	R-3m
lattice centering	F	P	R
crystal class	m-3m	6/mmm	-3m
crystal family	c	h	h*

* Lattice system is rhombohedral, crystal system is trigonal

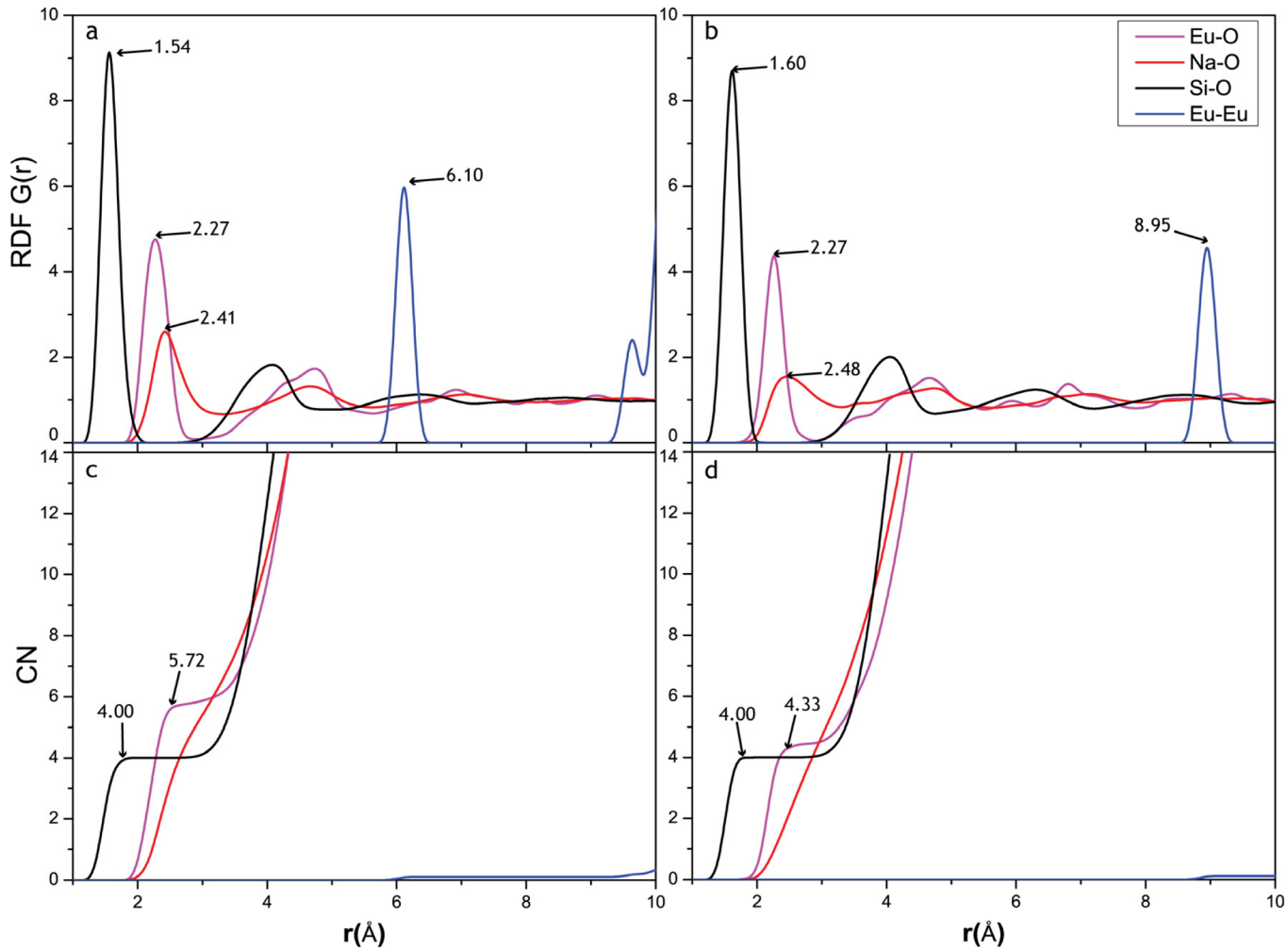
Lattice system vs crystal system, crystal family

space groups			lattice system	crystal family	crystal system
P1	...	P-1	anorthic*	a	anorthic
P2	...	C2/c	monoclinic	m	monoclinic
P222	...	Imma	orthorhombic	o	orthorhombic
P4	...	$I4_1/acd$	tetragonal	t	tetragonal
R3	...	R-3c	rhombohedral	**h**	trigonal
P3	...	P-3c1	**hexagonal**	**h**	**trigonal**
P6	...	$P6_3/mmc$	hexagonal	**h**	hexagonal
P23	...	Ia-3d	cubic	c	cubic

* anorthic is also called triclinic

Structure factor and radial distribution function

$$S(\boldsymbol{q}) = \frac{1}{N}\left|\sum_i \mathrm{e}^{-\mathrm{i}\boldsymbol{q}\boldsymbol{r}_i}\right| \equiv 1+\rho\int_V \mathrm{e}^{-\mathrm{i}\boldsymbol{q}\boldsymbol{r}} g(\boldsymbol{r})\,\mathrm{d}V,\; g(\boldsymbol{r}) = \sum_{i\neq 0}\delta\left(\boldsymbol{r}-\boldsymbol{r}_i\right)$$



Summary and Resources

See summary here

- Wikipedia
- Bilbao Crystallographic Server
- Crystal structures
- References: crystallography, symmetry
- Textbooks (sections General, Crystallography, Symmetry)

Visualization software:

- Jmol
- Mercury
- Surface explorer (online tool)