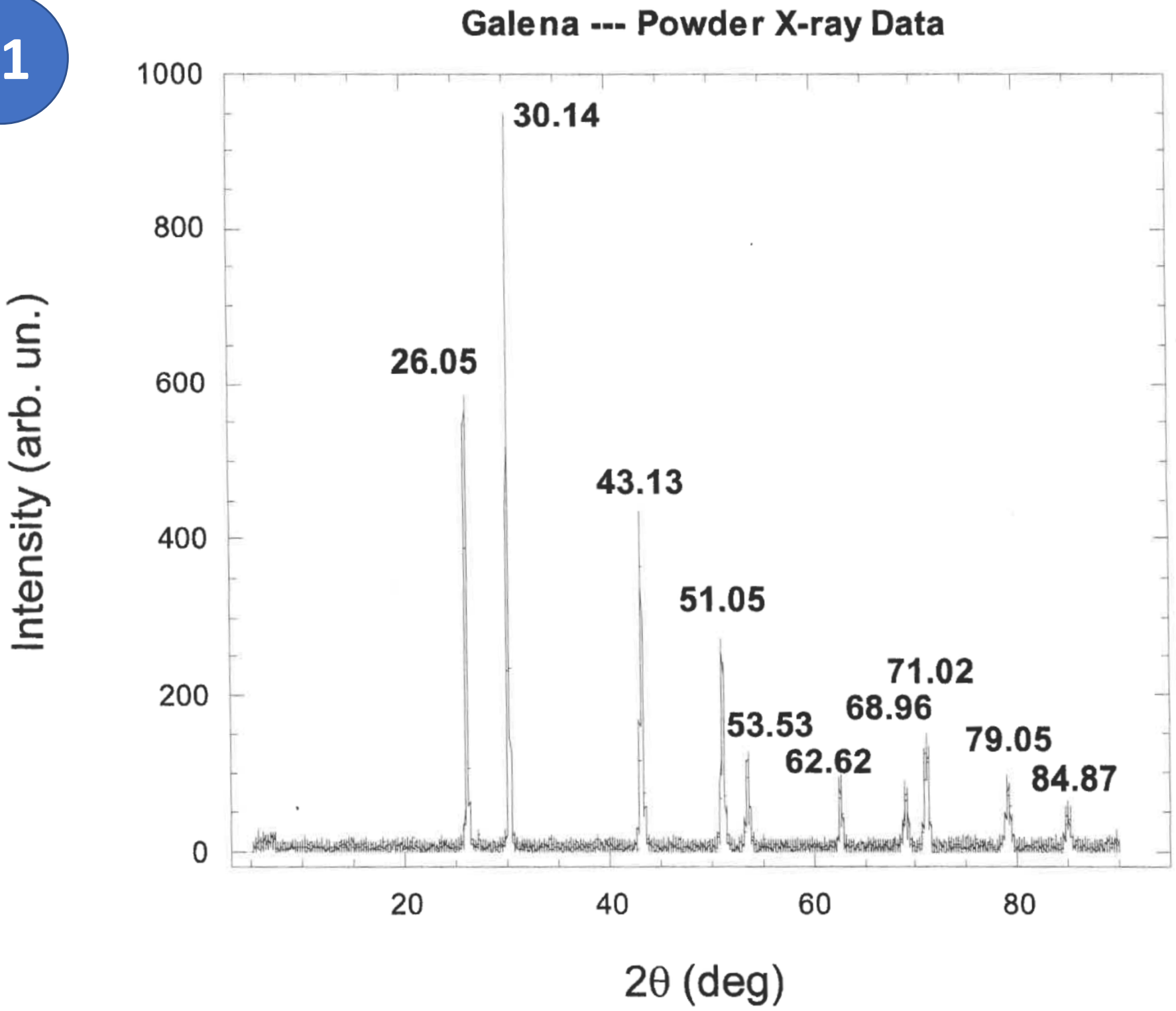
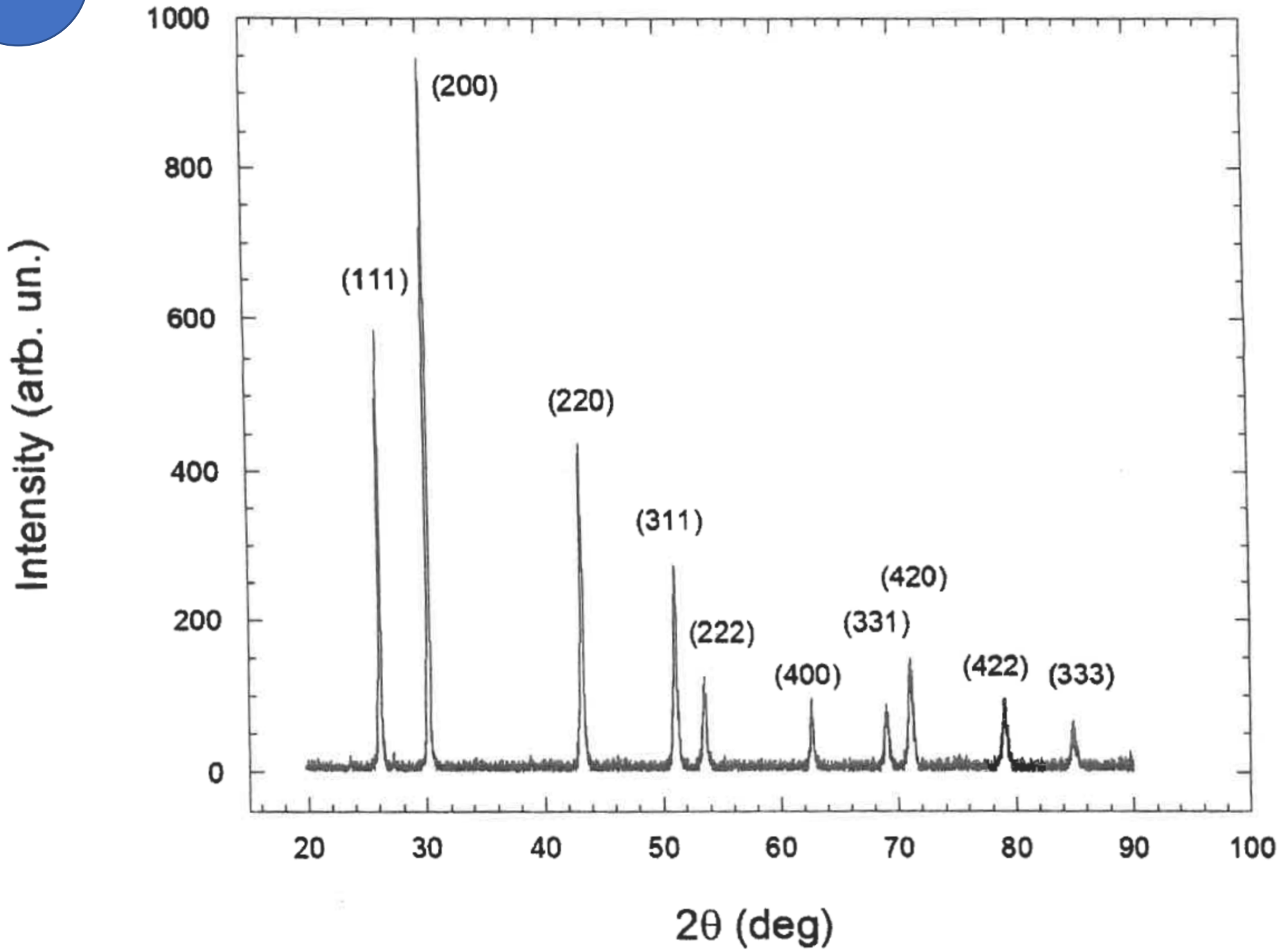
F1


Galena --- Powder X-ray Data
Intensity (arb. un.)
1000
800
600
400
200
0
20
40
60
80
2θ (deg)
30.14
26.05
43.13
51.05
53.53
62.62
68.96
71.02
79.05
84.87

F2


Intensity (arb. un.)
1000
800
600
400
200
0
(111)
(200)
(220)
(311)
(222)
(400)
(331)
(420)
(422)
(333)
20
30
40
50
60
70
80
90
100
2θ (deg)

F3

1st Course (*Física Básica Experimental 3*)
3rd Course (*F. Cuántica y Estr. de la Materia 2*)

CUBIC
a = b = c
α = β = γ = 90°

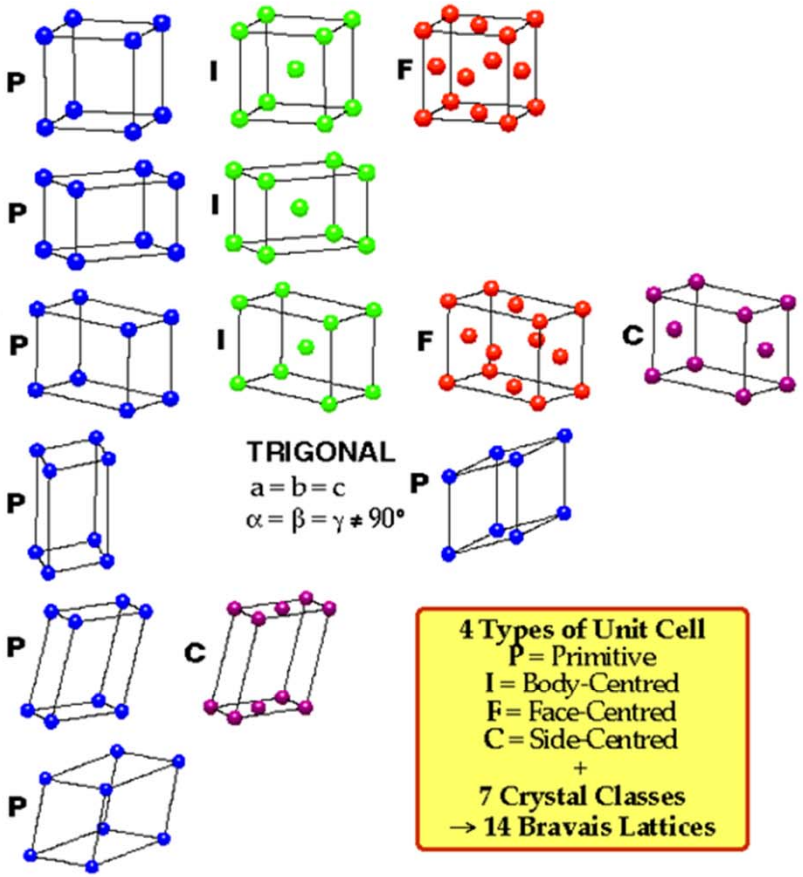
TETRAGONAL
a = b ≠ c
α = β = γ = 90°

ORTHORHOMBIC
a ≠ b ≠ c
α = β = γ = 90°

HEXAGONAL
a = b ≠ c
α = β = 90°
γ = 120°

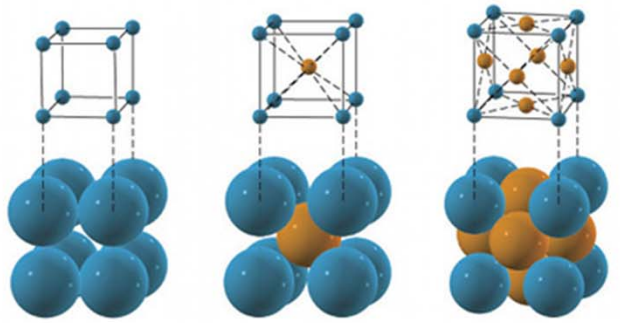
MONOCLINIC
a ≠ b ≠ c
α = γ = 90°
β ≠ 120°

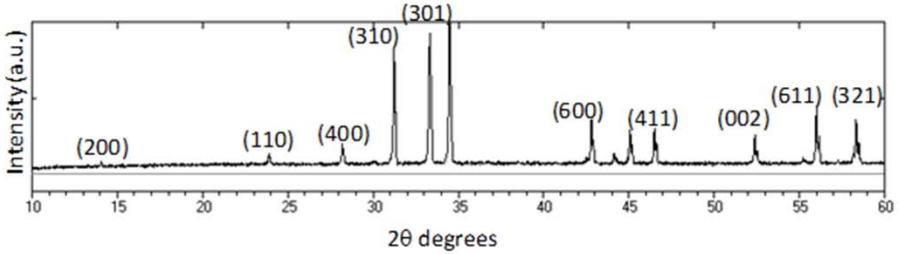
TRICLINIC
a ≠ b ≠ c
α ≠ β ≠ γ ≠ 90°



4 Types of Unit Cell
P = Primitive
I = Body-Centred
F = Face-Centred
C = Side-Centred
+
7 Crystal Classes
→ **14 Bravais Lattices**

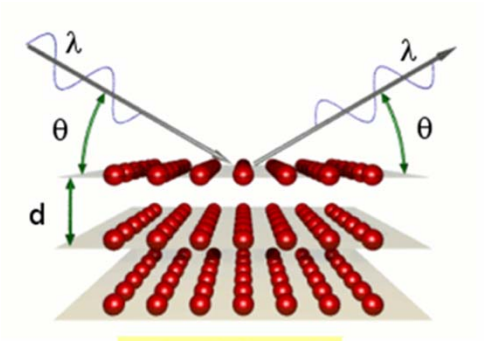
Simple (cubic) structures





n	2θ(°)	$\sin^2\theta$(°)	$\sin^2\theta_n/\sin^2\theta_1$	$3(\sin^2\theta n/\sin^2\theta_1)$	N	hkl
1	28.35	0.0600	1	3	3	**111**
2	32.68	0.0800	1.333	3.999	4	**200**
3	47.13	0.1598	2.663	7.989	8	**220**
4	55.91	0.2198	3.663	10.989	11	**311**
5	58.61	0.2396	3.993	11.979	12	**222**
6	68.86	0.3197	5.328	15.984	16	**400**
7	76.07	0.3796	6.327	18.981	19	**331**
8	78.39	0.3994	6.657	19.971	20	**420**
9	87.62	0.4792	7.987	23.961	24	**422**

F4



Bragg's Law

$$n\lambda = 2d\,\mathrm{sen}\theta$$

Peaks Position

System	d_{hkl}
Cubic	$\left[\frac{1}{a^2}(h^2+k^2+l^2)\right]^{-1/2}$
Tetragonal	$\left[\frac{h^2+k^2}{a^2}+\frac{l^2}{c^2}\right]^{-1/2}$
Orthorhombic	$\left[\frac{h^2}{a^2}+\frac{k^2}{b^2}+\frac{l^2}{c^2}\right]^{-1/2}$
Hexagonal	$\left[\frac{4}{3a^2}(h^2+hk+k^2)+\frac{l^2}{c^2}\right]^{-1/2}$ hexagonal indexing $\left[\frac{1}{a^2}\frac{(h^2+k^2+l^2)\sin^2\alpha+2(hk+kl+lh)(\cos^2\alpha-\cos\alpha)}{1-2\cos^3\alpha+3\cos^2\alpha}\right]^{-1/2}$ rhombohedral indexing
Monoclinic	$\left[\frac{h^2}{a^2}+\frac{l^2}{c^2}-\frac{2hl\cos\beta}{ac}}{\sin^2\beta}+\frac{k^2}{b^2}\right]^{-1/2}$
Triclinic	$\left[\frac{\frac{h^2}{a^2}\sin^2\alpha+\frac{k^2}{b^2}\sin^2\beta+\frac{l^2}{c^2}\sin^2\gamma+\frac{2hk}{ab}(\cos\alpha\cos\beta-\cos\gamma)+\frac{2kl}{bc}(\cos\beta\cos\gamma-\cos\alpha)+\frac{2lh}{ca}(\cos\gamma\cos\alpha-\cos\beta)}{1-\cos^2\alpha-\cos^2\beta-\cos^2\gamma+2\cos\alpha\cos\beta\cos\gamma}\right]^{-1/2}$

Cubic Structure

$$\frac{1}{d_{hkl}^2}=\frac{h^2+k^2+l^2}{a^2}$$

n	Sym.	Q(khl;ABCDEF)	short	relation to a,c,b
:***1***	*cubic*	$q^2 = [h^2+k^2+l^2].A$	$Q = [M^2].A$	$a=(2\pi)/\sqrt{A}$;
:***2***:	*tetragonal*:	$q^2 = [h^2+k^2].A + [l^2].C$	$Q = [HK].A+[L^2].C$	$a=(2\pi)/\sqrt{A}$; $c=(2\pi)/\sqrt{C}$
:***2***:	*hexagonal*:	$q^2 = [h^2+k^2+h.k].A + [l^2].C$	$Q = [HK].A+[L^2].C$	$a=(4\pi)/\sqrt{(3A)}$; $c=(2\pi)/\sqrt{C}$
:***3***:	*orthorhombic*:	$q^2 = [h^2]A + [k^2]B + [l^2].C$		$a=(2\pi)/\sqrt{A}$; $b=(2\pi)/\sqrt{B}$; $c=(2\pi)/\sqrt{C}$
:***4***:	*monoclinic*:	$q^2 = [h^2]A + [k^2]B + [l^2].C + [h.l].D$		$a.\sin\beta=(2\pi)/\sqrt{A}$; $b=(2\pi)/\sqrt{B}$; $c.\sin\beta=(2\pi)/\sqrt{C}$; $\cos\beta= -D/2\sqrt{(AC)}$
:***6***:	*triclinic*:	$q^2 = [h^2]A + [k^2]B + [l^2].C + [h.l].D + [h.k].E + [k.l].F$		(see Cullity page 501)

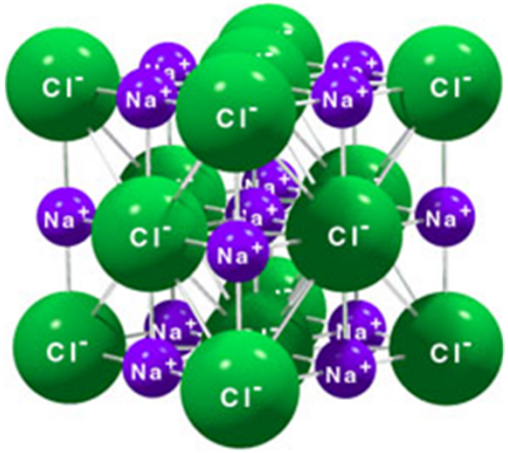
F5

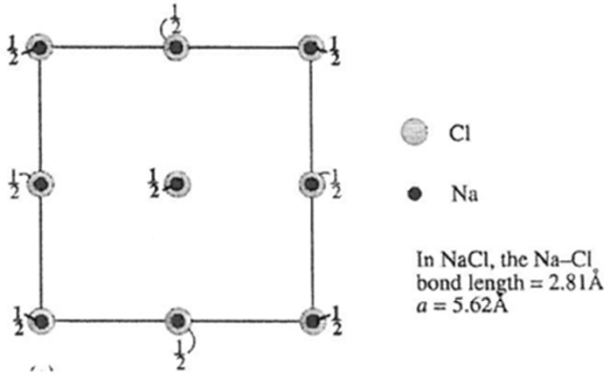
General rules for systematic absences due to lattice type (for <u>all</u> crystal systems)

Lattice	Restrictions on *hkl*
P	None
A	$(k + l)$ odd **absent**
B	$(h + l)$ odd **absent**
C	$(h + k)$ odd **absent**
I	$(h + k + l)$ odd **absent**
F	h, k, and l not all odd or all even, **absent**

Warning: Some reflections may be missing for reasons not connected with lattice type. The opposite of systematic absence is not systematic presence!

F6





F Lattice

Motif: Cl: 0,0,0; Na: 0,0,1/2

$$F_{hkl} = \sum_{j=1}^{n} f_j e^{[2\pi i(hx_j+ky_j+lz_j)]}$$

$$F_{hkl} = \sum_{j=1}^{n} f_j\left[cos2\pi(hx_j + ky_j + lz_j) + isen2\pi(hx_j + ky_j + lz_j)\right]$$

Calculation of structure factor for the 331 reflection:

$$F_{hkl} = \sum_{j=1}^{j=n} f_j\left[\cos 2\pi\left(hx_j + ky_j + lz_j\right) + i\sin 2\pi\left(hx_j + ky_j + lz_j\right)\right]$$

$$F_{331} = 4f_{Na}\left[\cos 2\pi\left(3\times 0 + 3\times 0 + 1\times \tfrac{1}{2}\right) + i\sin 2\pi\left(3\times 0 + 3\times 0 + 1\times \tfrac{1}{2}\right)\right]$$

$$+4f_{Cl}\left[\cos 2\pi(3\times 0 + 3\times 0 + 1\times 0) + i\sin 2\pi(3\times 0 + 3\times 0 + 1\times 0)\right]$$

$$= 4\left[f_{Cl} - f_{Na}\right]$$

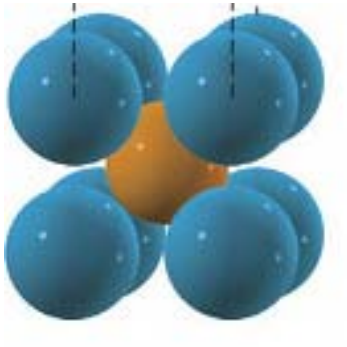
Multiplicity of 331 planes: $m_{331} = 24$

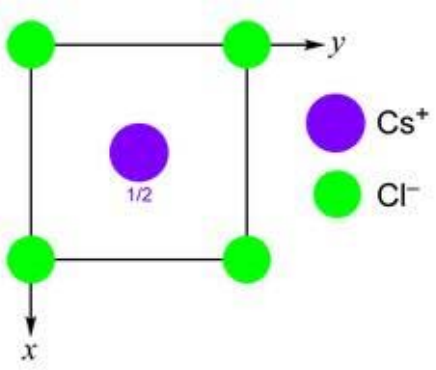
Calculation of intensity of 331 reflection:

$$I_{331} \propto G(\theta).m_{331}.|F_{331}|^2 \propto 24\times 16\left[f_{Cl} - f_{Na}\right]^2$$

F7

Cesium Chloride





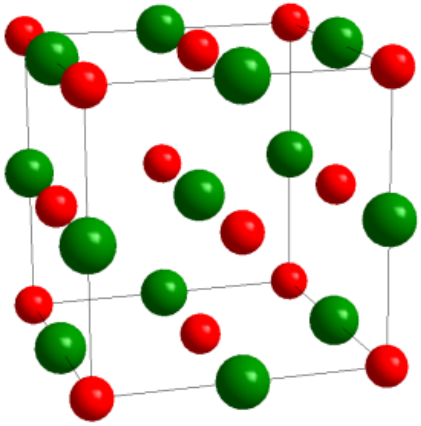
CsCl

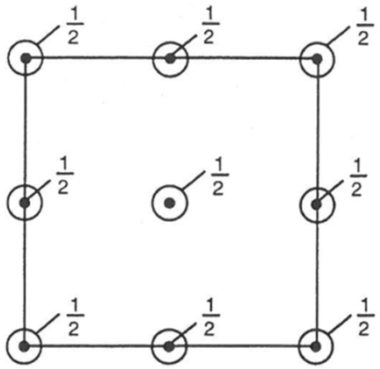
Motif:

Cl (0,0,0)

Cs (1/2,1/2, 1/2)

Rock salt





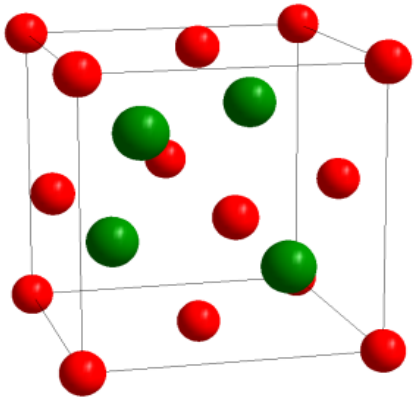
NaCl

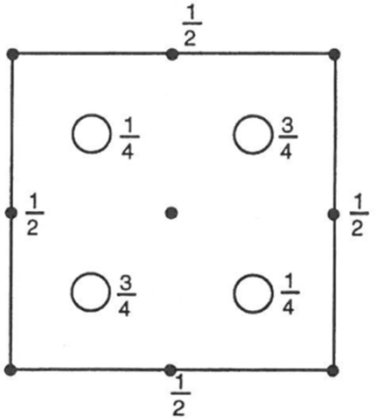
Motif:

Na (0,0,0)

Cl (1/2,0,0)

Zincblende





ZnS

Motif:

Zn (0,0,0)

S (1/4, 1/4, 1/4)