Crystal structures

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The simplest crystal structures, including of most elements, can be considered as formed from the close packings of spheres. Studying the close-packing of spheres throws light on the kind of criteria that are important for stabilizing some structures over others.

- Close packing of spheres — ccp and hcp
- The sizes of tetrahedral and octahedral voids and the notion of radius ratio (see handout)
- The structures of the elements:
  - α-Po at 283 K:
    SG = $Pm\overline{3}m$ (No. 221) a = 3.295 Å

Atom	x	y	z
Po	0	0	0

  - α-Fe (bcc-Fe):
    SG = $Im\overline{3}m$ (No. 229) a = 2.86 Å

Atom	x	y	z
Fe	0	0	0

  - Cu:

    SG = $Fm\overline{3}m$ (No. 225) a = 3.60 Å

Atom	x	y	z
Cu	0	0	0

  - Mg:

    SG = $P6_3/mmc$ (No. 194) a = 3.20 Å c = 5.20 Å

Atom	x	y	z
Mg	1/3	2/3	3/4

  - Si:

    SG = $Fd\overline{3}m$ (No. 227) a = 5.43042 Å

Atom	x	y	z
Si	0	0	0

  - C (graphite):

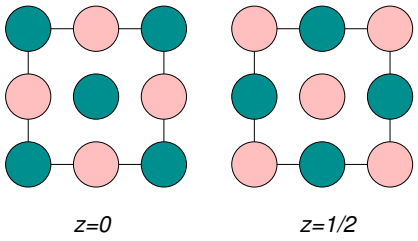
    SG = $P6_3/mmc$ (No. 194) a = 2.4612 Å c = 6.7090 Å

Atom	x	y	z
C	0	0	1/4
C	2/3	1/3	1/4

- AB crystal structures (NaCl, CsCl, ZnS (wurtzite), ZnS (zinc blende) NiAs)

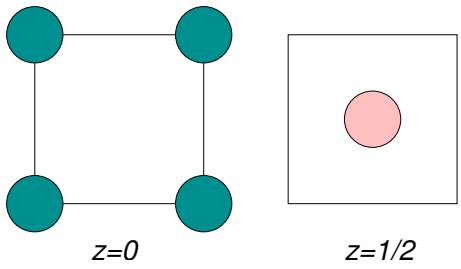
NaCl: SG = $Fm\bar{3}m$ (No. 225) $a = 5.63$ Å

Atom	x	y	z
Na	0	0	0
Cl	1/2	1/2	1/2



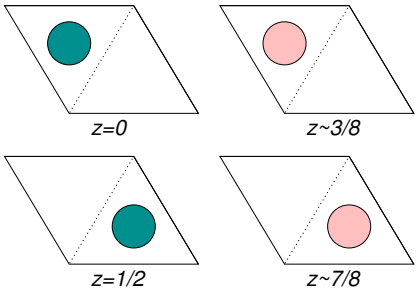
CsCl: SG = $Pm\bar{3}m$ (No. 229) $a = 4.11$ Å

Atom	x	y	z
Cs	1/2	1/2	1/2
Cl	0	0	0



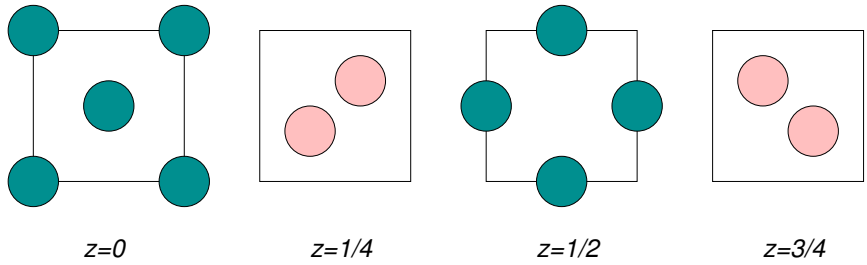
ZnS (wurtzite): SG = $P6_3mc$ (No. 186) $a = 3.83$ Å $= 6.23$ Å

Atom	x	y	z
Zn	2/3	1/3	0
S	2/3	1/3	∼3/8



ZnS (zinc blende): SG = $F\bar{4}3m$ (No. 216) $a = 5.41$ Å

Atom	x	y	z
Zn	0	0	0
S	1/4	1/4	1/4



NiAs: SG = $P6_3/mmc$ (No. 194) $a = 3.60$ Å $c = 5.01$

Atom	x	y	z
Ni	0	0	0
As	2/3	1/3	1/4