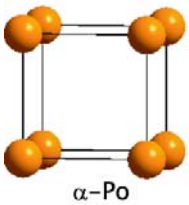
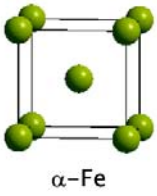
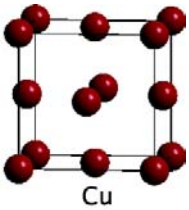
Class 1: Simple structures



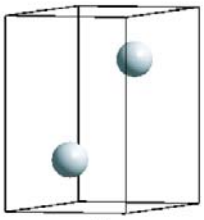
α–Po



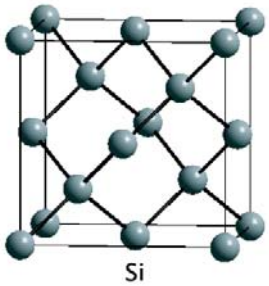
α–Fe



Cu

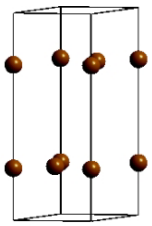


Mg

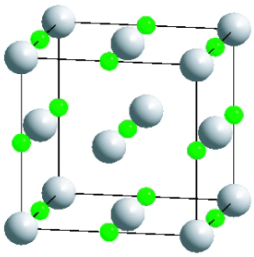


Si

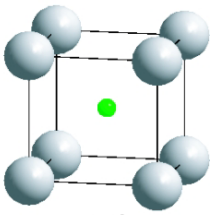
Class 1: Simple structures p2



C (graphite)



NaCl



CsCl

Class 1: Simple structures p3

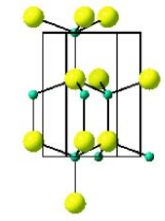
Use of the International Tables:
The example of space group *Fd-3m* (No. 227)

Origin Choice 1 (at -1/8, -1/8, -1/8)
Coordinates: (0,0,0)+ (0,1/2,1/2)+ (1/2,0,1/2)+ (1/2,1/2,0)+

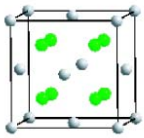
16	d	-3m	5/8,5/8,5/8	3/8,7/8,1/8 ...
8	a	-43m	0,0,0	3/4,1/4,3/4

Structure of Diamond Si: *Fd-3m* Si at 0,0,0 a = 5.43042 Å

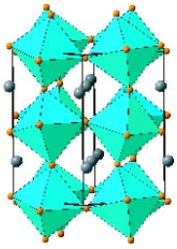
Class 1: Simple structures p4



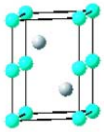
ZnS wurtzite



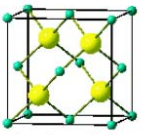
Fluorite



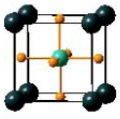
Perovskite
$CaTiO_3$



NiAs



ZnS zinc blende



cubic perovskite ($BaSnO_3$)

Class 1: Simple structures p5

Stabilization of ionic crystals:

$$-N_A \sum \frac{q_1 q_2 e^2}{4\pi\varepsilon_0 r_{ij}}$$ ionic, also: $$E_C = -AN_A q_1 q_2 \frac{e^2}{4\pi\varepsilon_0 R}$$

$$-N_A \sum B_{ij} \exp(-\alpha_{ij} r_{ij})$$ repulsion

$$+N_A \sum C_{ij} r_{ij}^{-6}$$ dispersion

$$-2N_A \frac{1}{2} h\nu_{\max}$$ zero point

Madelung constants:
A = 1.76267 (CsCl)
A = 1.74756 (NaCl)
A = 1.64132 (wurtzite)
A = 1.63805 (blende)

Class 1: Simple structures p6

Paulings rules (approximately):

1. *Coordination Polyhedra*: ... of anions fromed around cations. Cation-anion distances are determined by the sum of the radii, and corrdination number by the radius ratio.
2. *Electrostatic valence rule:* In a stable ionic structure, the valence (ionic charge) of each anion with changed sign is exactly equal to the sum of the electrostatic bond strengths to it from adjacent cations. The electrostatic bond strength is defined as ratio of charge on cation to its coordination number.
3. *Linking of polyhedra:* The presence of shared edges and especially of shared faces decreases stability. The effect is large for cations with high charge and low coordination number.
4. *Sharing of anions:* Polyhedra around cations with high charge and low coordination number tend not to share features.
5. *Parsimony:* Structures tend to be simple