

Visualizing important crystal structures

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Further notes on understanding the International Tables

$Cmm2$

C_{2v}^{11}

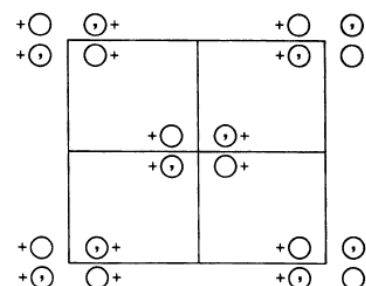
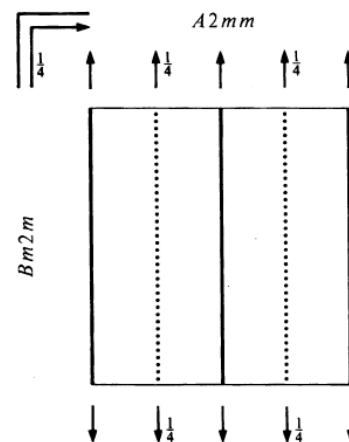
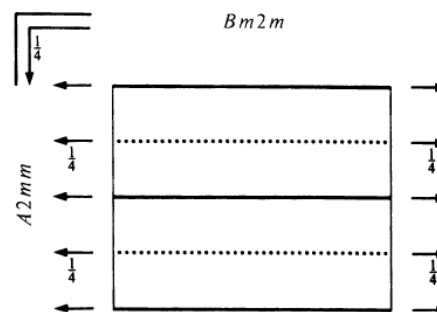
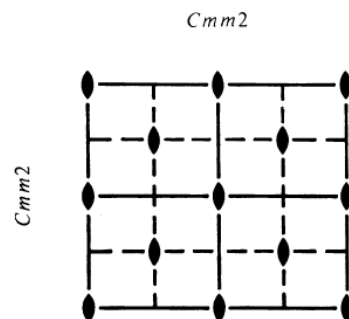
$mm2$

Orthorhombic

No. 35

$Cmm2$

Patterson symmetry $Cmmm$



Origin on $mm2$

Asymmetric unit $0 \leq x \leq \frac{1}{4}; 0 \leq y \leq \frac{1}{2}; 0 \leq z \leq 1$

Symmetry operations

For $(0,0,0)+$ set

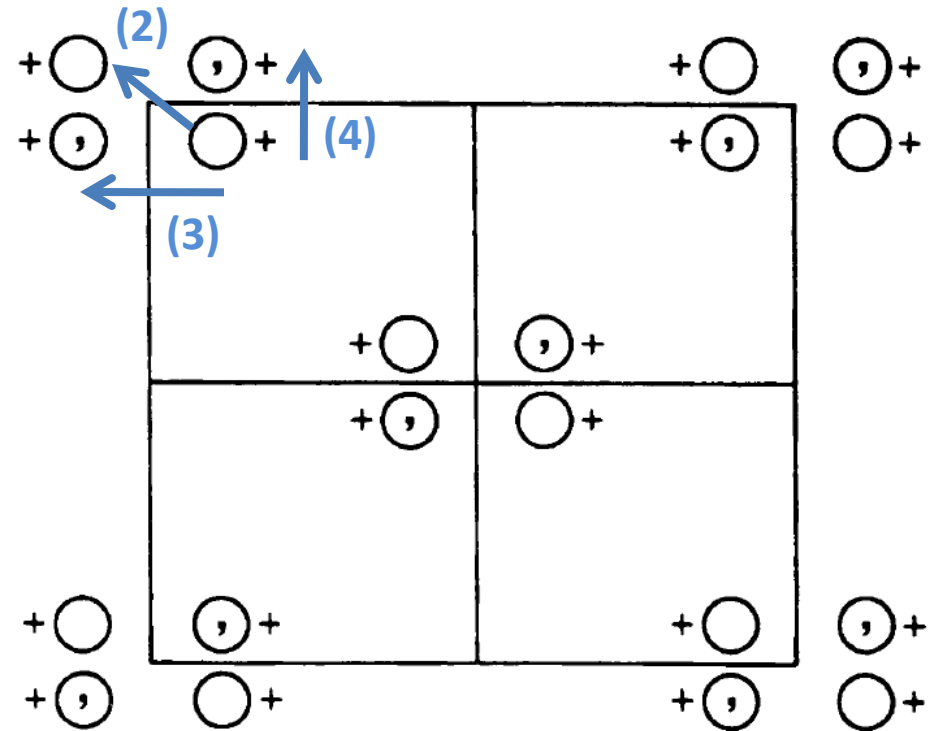
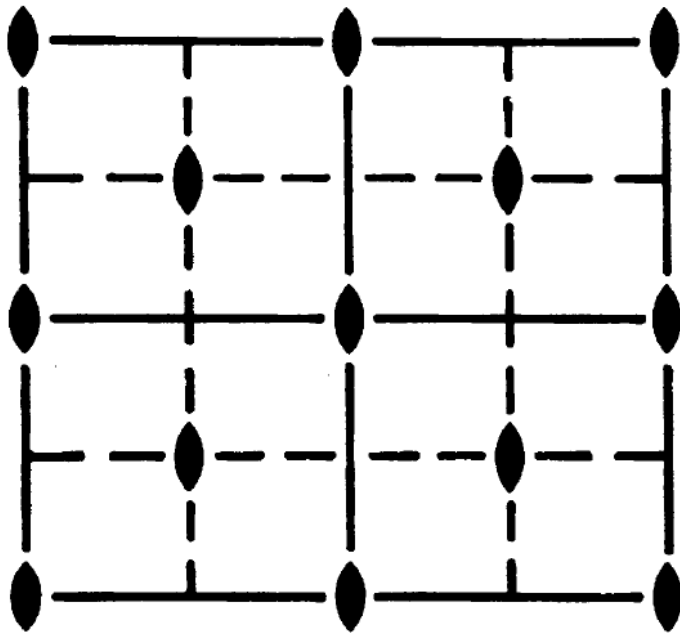
(1) 1 (2) $2 \ 0,0,z$ (3) $m \ x,0,z$ (4) $m \ 0,y,z$

For $(\frac{1}{2},\frac{1}{2},0)+$ set

(1) $t(\frac{1}{2},\frac{1}{2},0)$ (2) $2 \ \frac{1}{4},\frac{1}{4},z$ (3) $a \ x,\frac{1}{4},z$ (4) $b \ \frac{1}{4},y,z$

Symmetry operations

C_{2v}



Symmetry operations

For $(0,0,0)+$ set

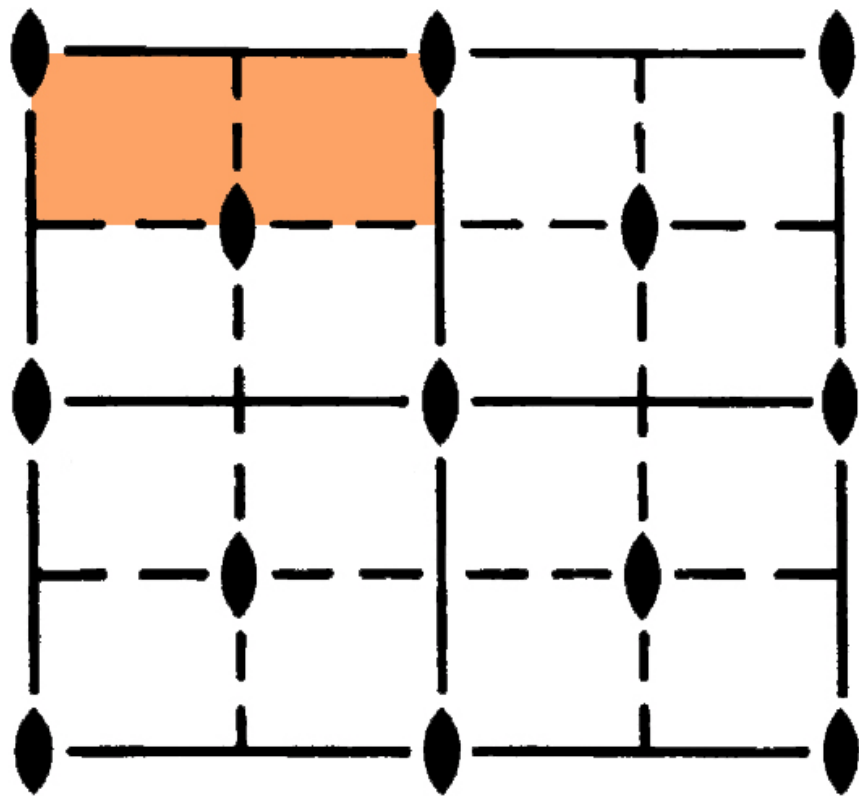
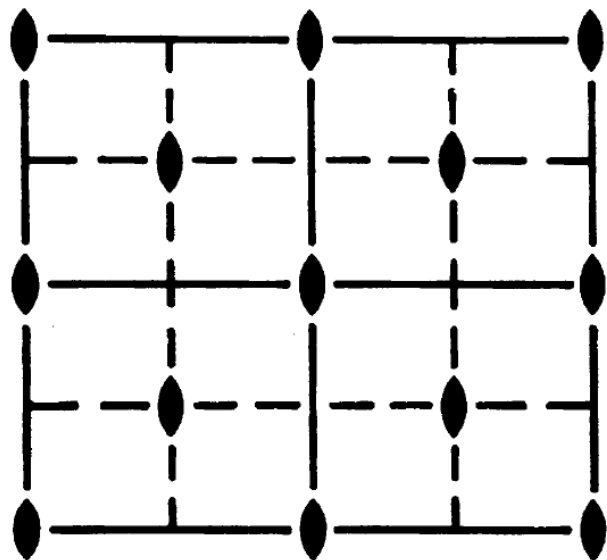
- | | | | |
|-------|---------------|-----------------|-----------------|
| (1) 1 | (2) 2 $0,0,z$ | (3) m $x,0,z$ | (4) m $0,y,z$ |
|-------|---------------|-----------------|-----------------|

For $(\frac{1}{2},\frac{1}{2},0)+$ set

- | | | | |
|------------------------------------|-----------------------------------|---------------------------|---------------------------|
| (1) $t(\frac{1}{2},\frac{1}{2},0)$ | (2) 2 $\frac{1}{4},\frac{1}{4},z$ | (3) a $x,\frac{1}{4},z$ | (4) b $\frac{1}{4},y,z$ |
|------------------------------------|-----------------------------------|---------------------------|---------------------------|

Asymmetric Unit

C_{2v}



Asymmetric unit

$$0 \leq x \leq \frac{1}{4}; \quad 0 \leq y \leq \frac{1}{2}; \quad 0 \leq z \leq 1$$

Wyckoff positions

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

Reflection conditions

$(0,0,0)+ (\frac{1}{2},\frac{1}{2},0)+$

General:

8 f 1 (1) x,y,z (2) \bar{x},\bar{y},z (3) x,\bar{y},z (4) \bar{x},y,z

$hkl : h+k=2n$

$0kl : k=2n$

$h0l : h=2n$

$hkl : h+k=2n$

$h00 : h=2n$

$0k0 : k=2n$

Special: as above, plus

4 e $m..$ $0,y,z$ $0,\bar{y},z$

no extra conditions

4 d $.m.$ $x,0,z$ $\bar{x},0,z$

no extra conditions

4 c $..2$ $\frac{1}{4},\frac{1}{4},z$ $\frac{1}{4},\frac{3}{4},z$

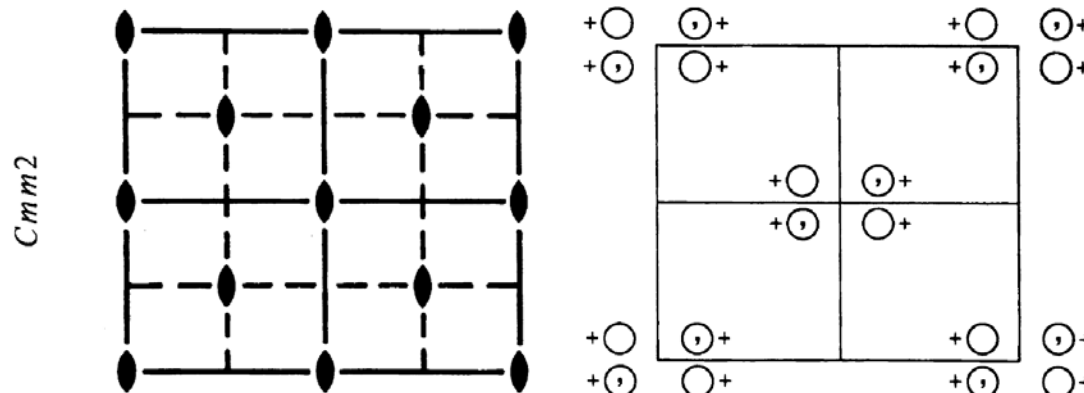
$hkl : h=2n$

2 b $mm2$ $0,\frac{1}{2},z$

no extra conditions

2 a $mm2$ $0,0,z$

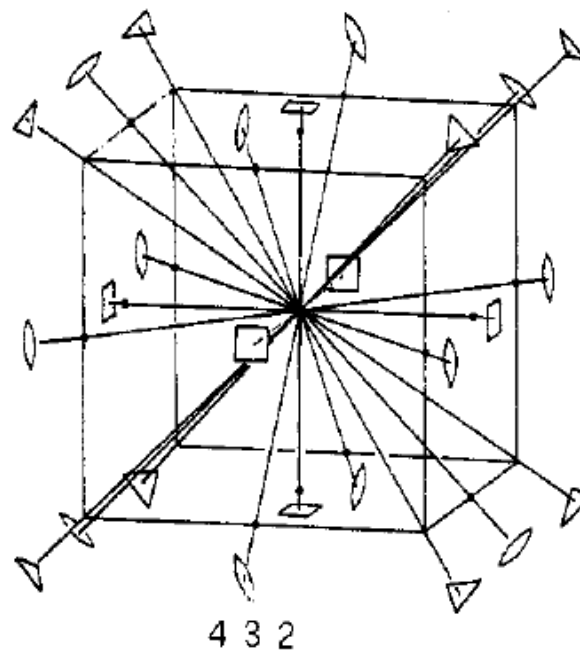
no extra conditions



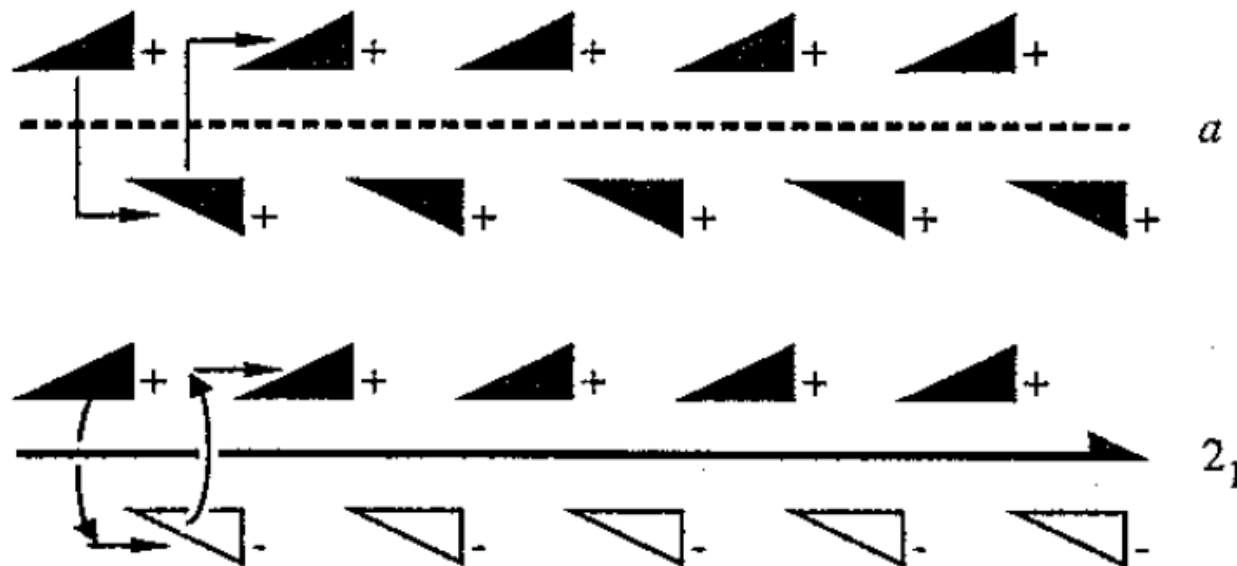
Nomenclature of space groups

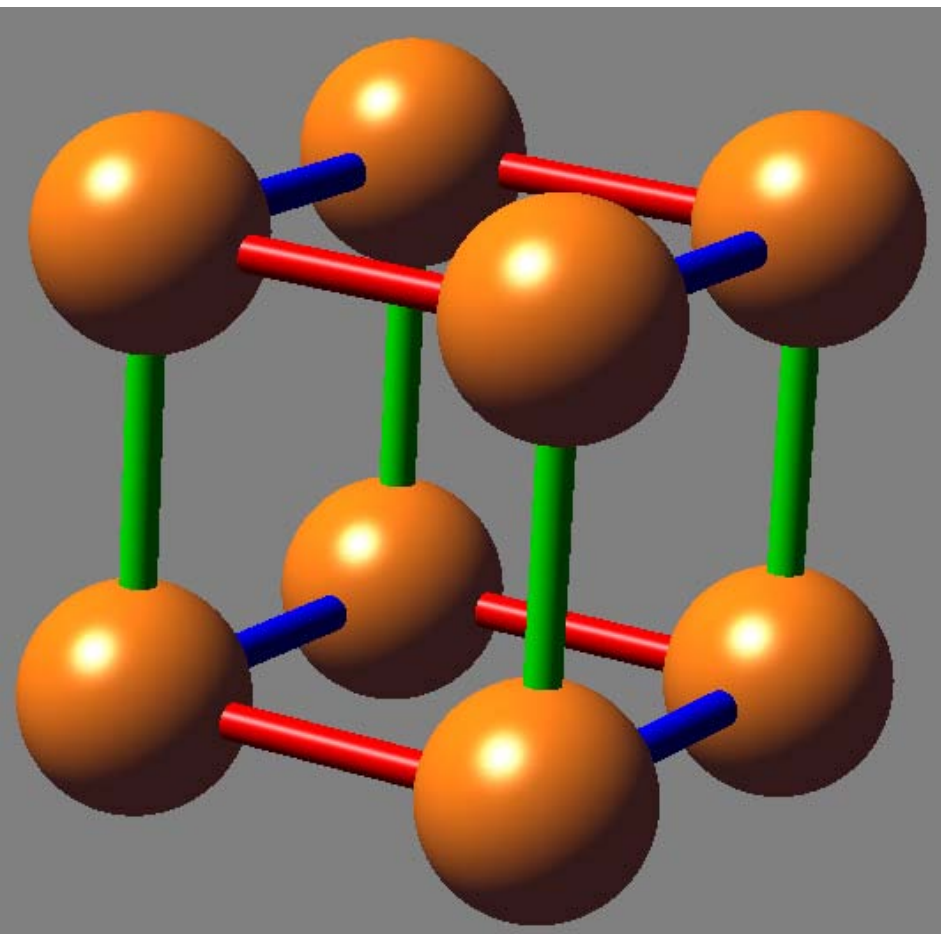
Crystal system	Example	Explanation
Triclinic	$P1, P\bar{1}$	Only center of inversion is possible
Monoclinic	$C2, P2_1/m$	Only twofold symmetry in one direction (y) is possible
Orthorhombic	$P222_1, Fdd2$	Twofold symmetry along x , then y , then z
Tetragonal	$P4_3, I4_1/amd$	Fourfold symmetry along z , then x (y), then <i>xy</i> diagonal
Trigonal	$P3_212, P\bar{3}m2$	Threefold symmetry along z , then x (y), then <i>xy</i> diagonal
	$R3, R\bar{3}2$	Threefold symmetry along space diagonal, then perpendicular to it
Hexagonal	$P6_2, P6/mcc$	Sixfold symmetry along z , then x (y), then <i>xy</i> diagonal
Cubic	$P2_13, F432$	Symmetry along x (y , z), then threefold space diagonals, then face diagonals

Ordering of axes in the cubic point group and space group nomenclature

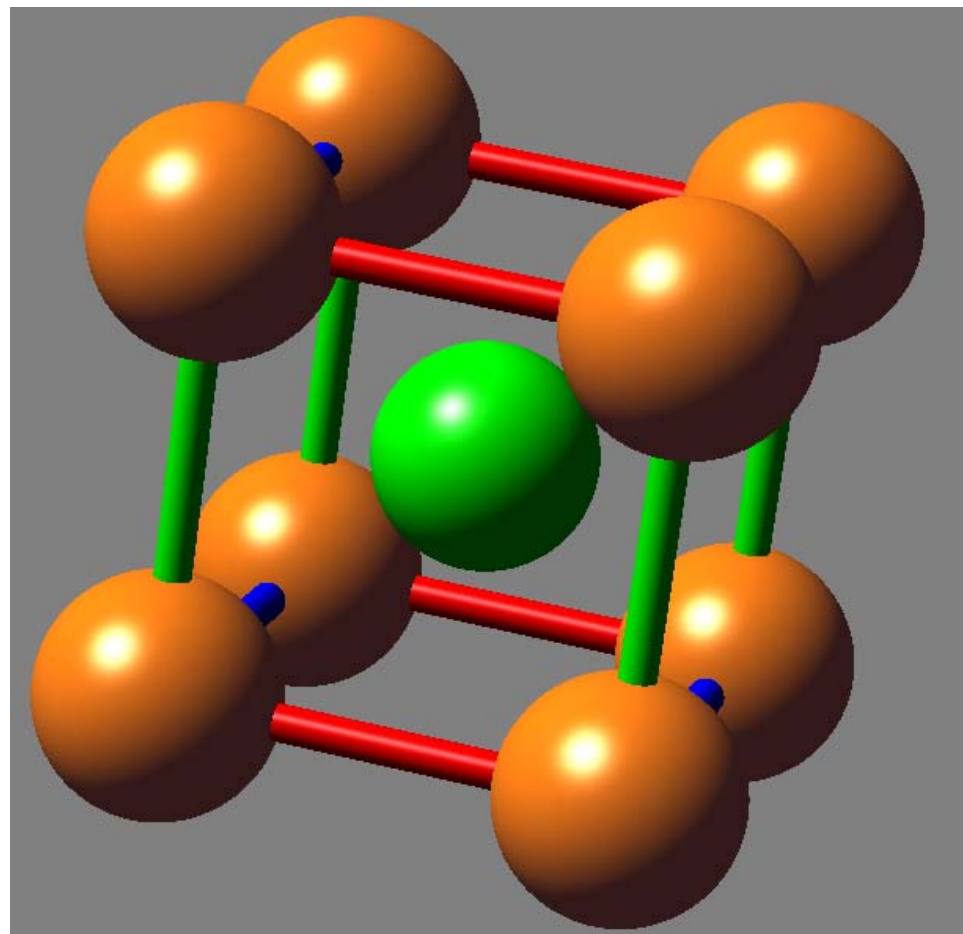


Comparison of screw and glide



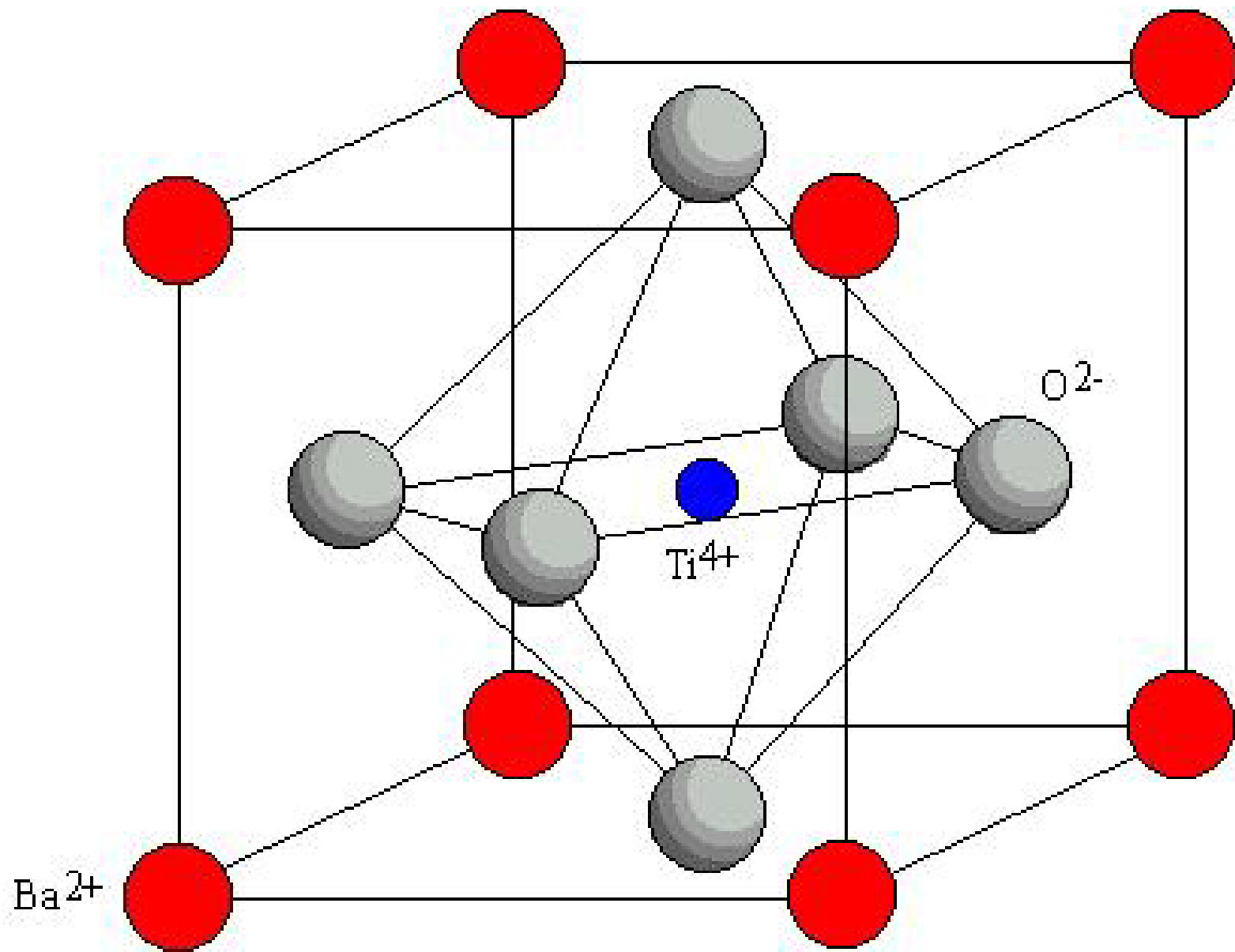


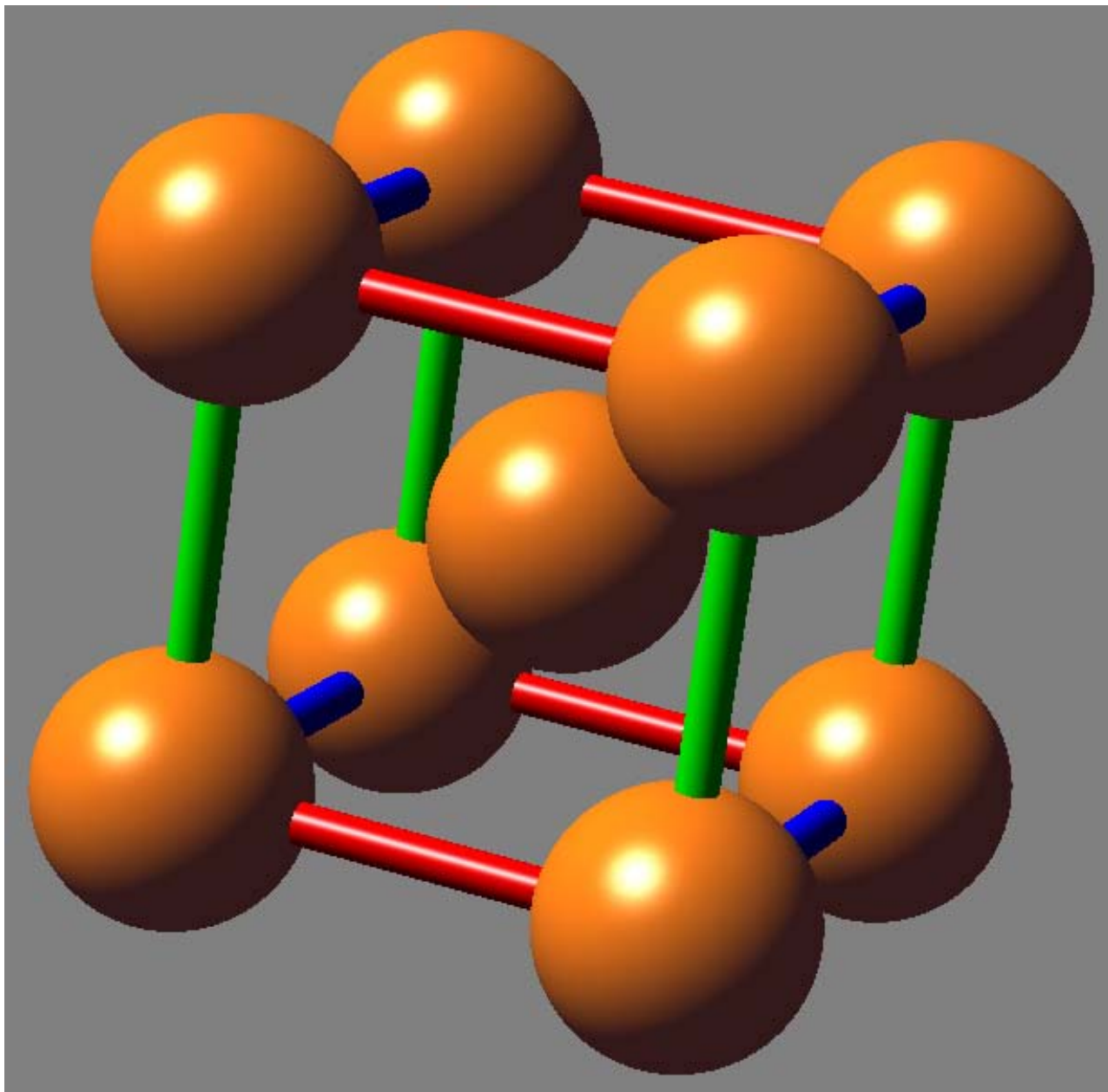
Po



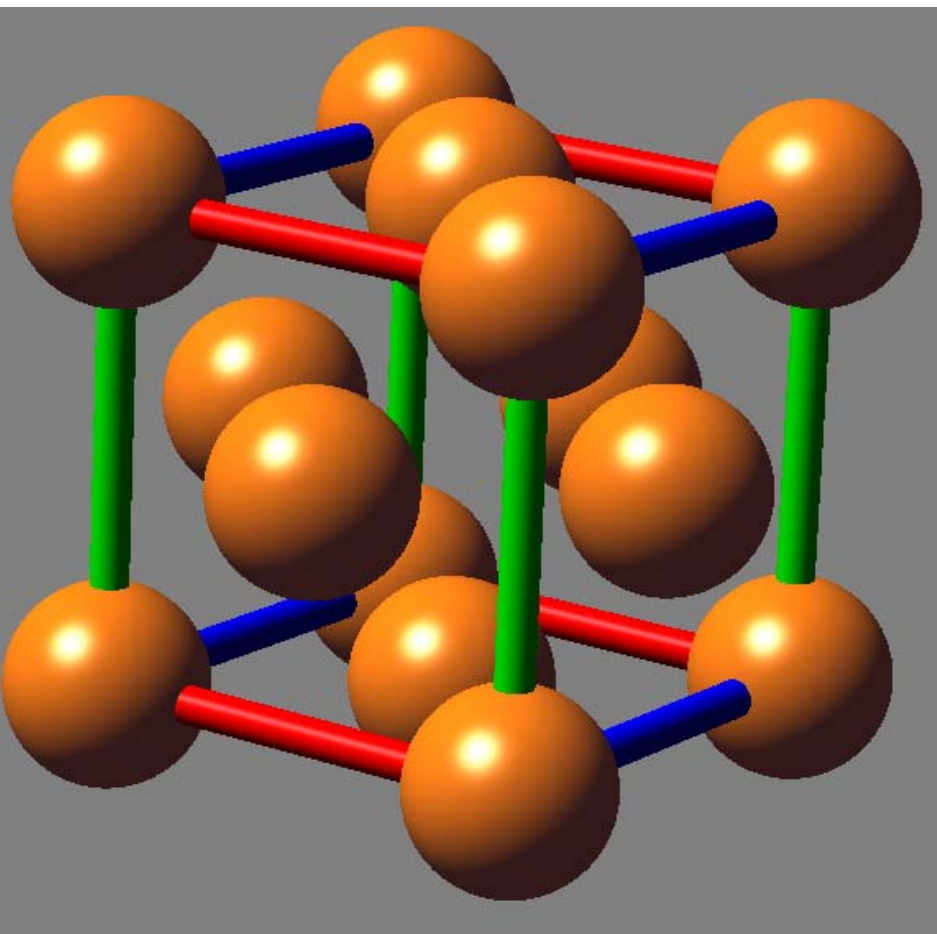
CsCl

$Pm\bar{3}m$

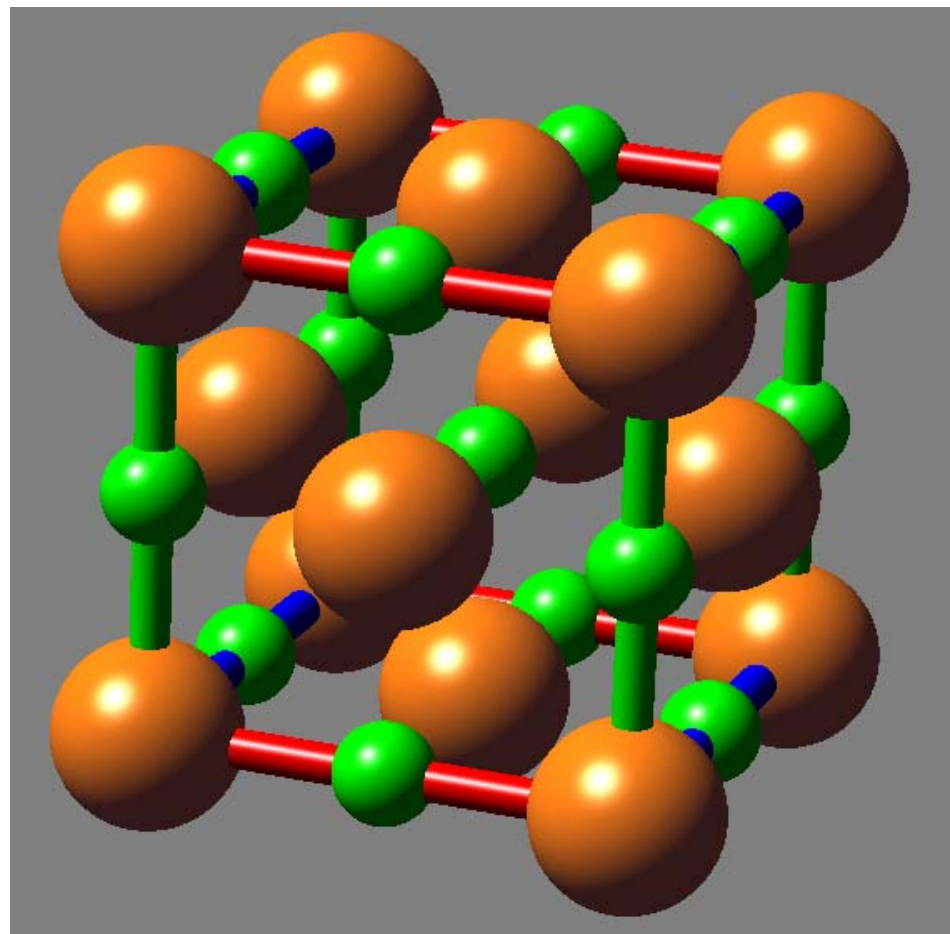




Fe $\overline{Im3m}$

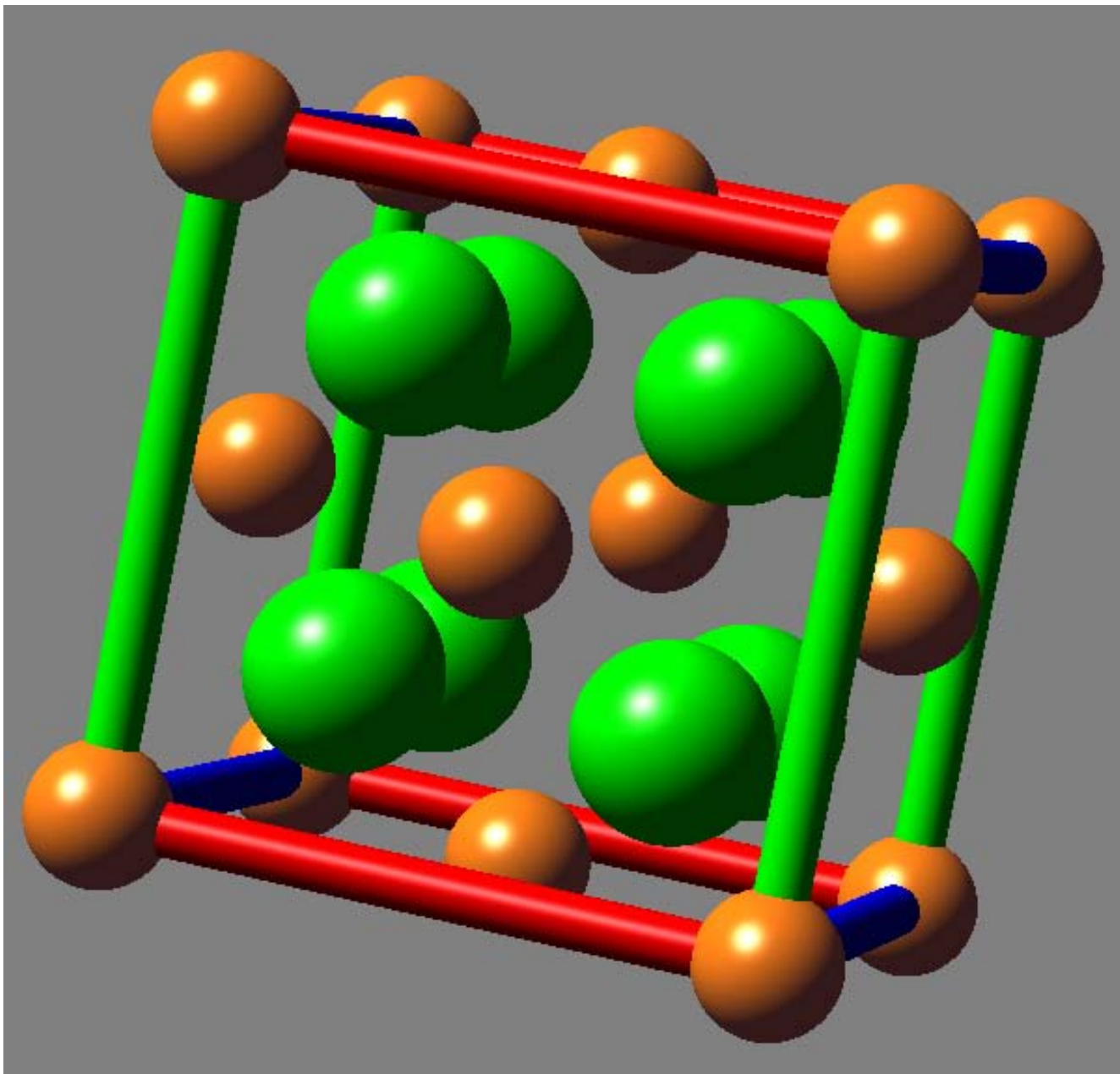


Cu

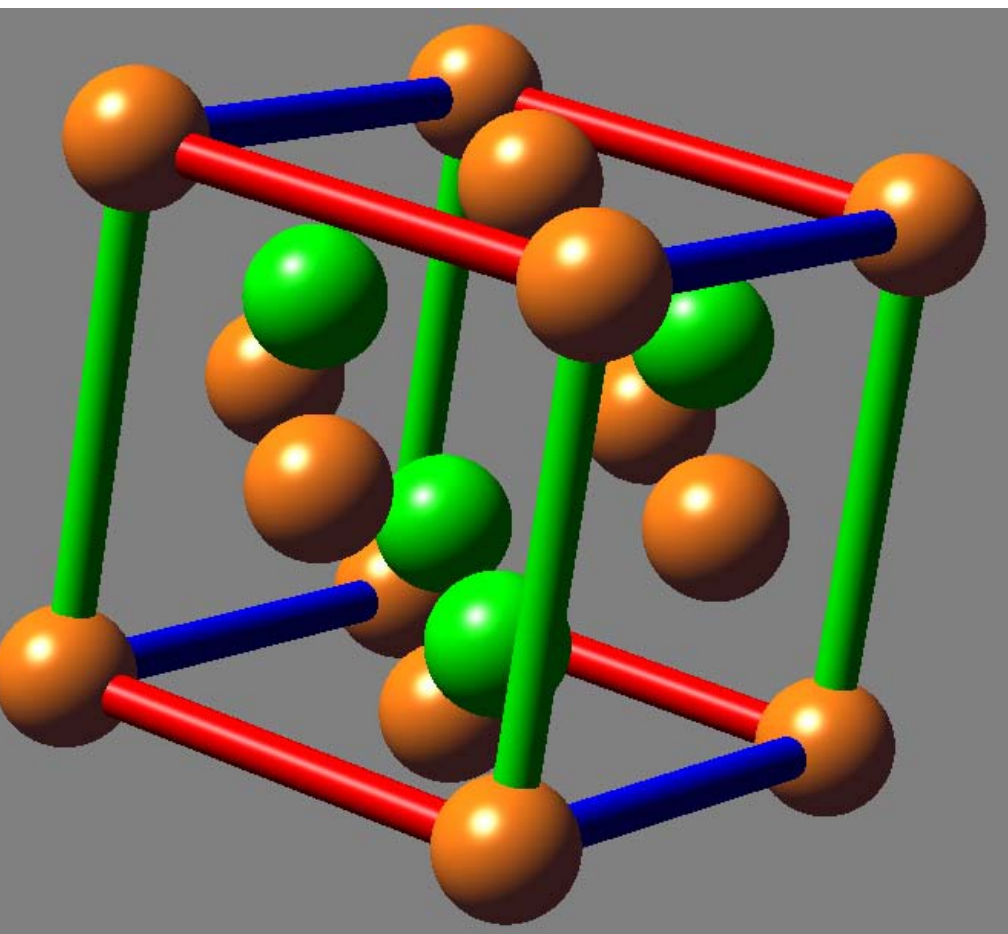


NaCl

$Fm\bar{3}m$

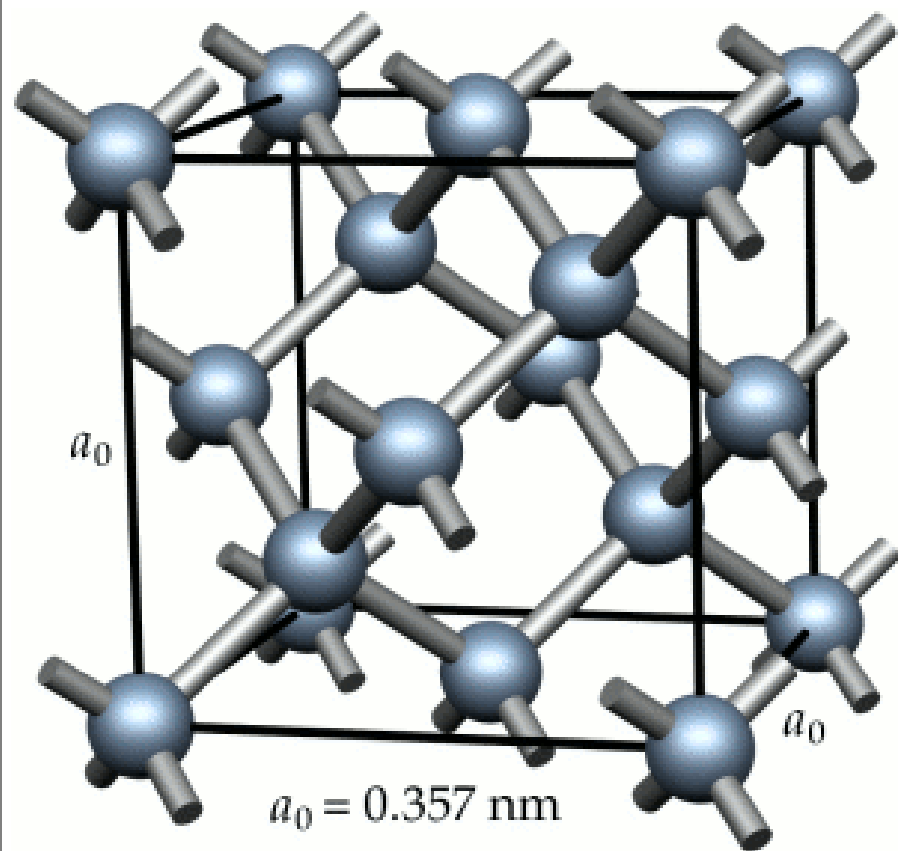


CaF_2 $\overline{Fm3m}$

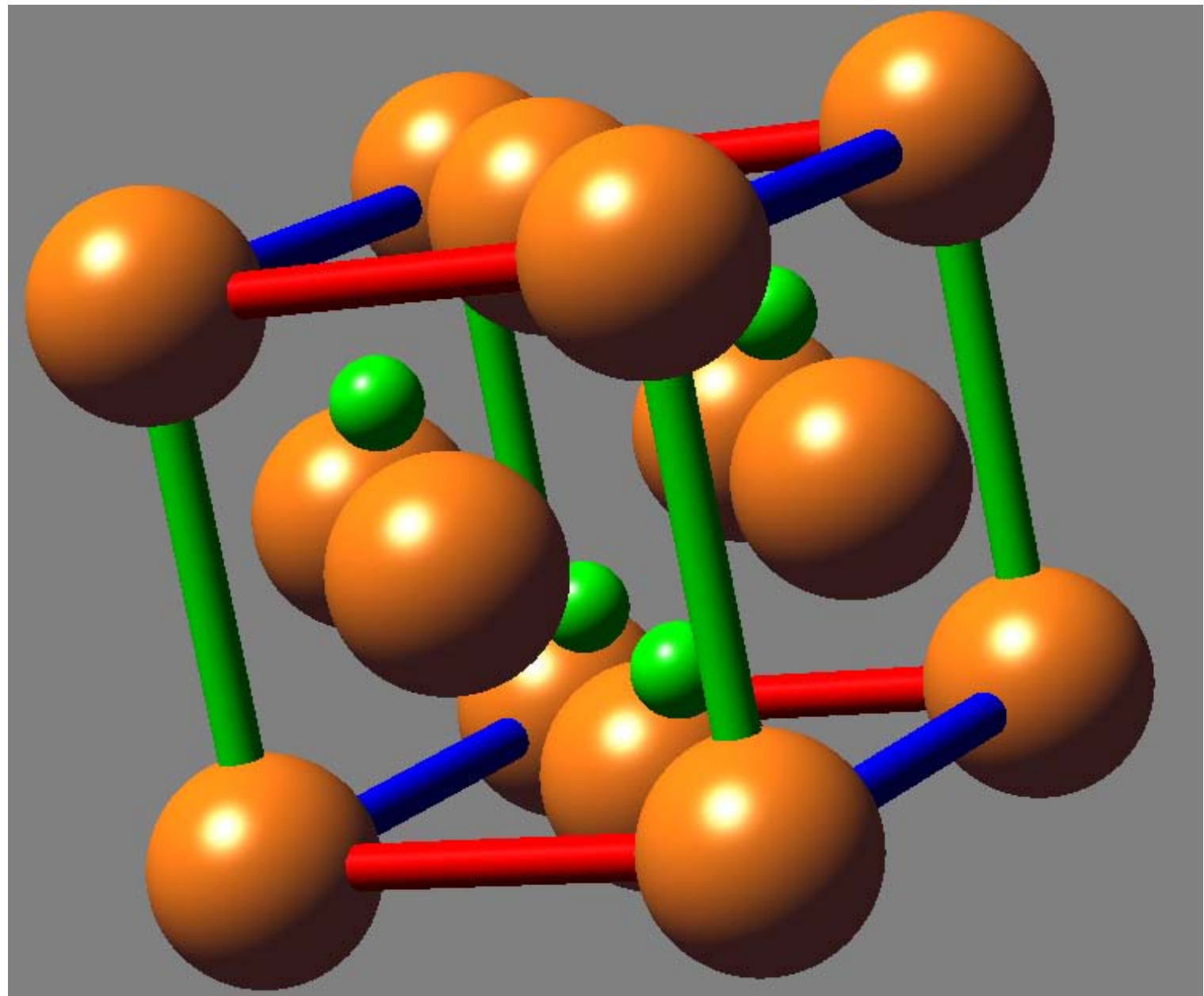


Diamond

$Fd\bar{3}m$

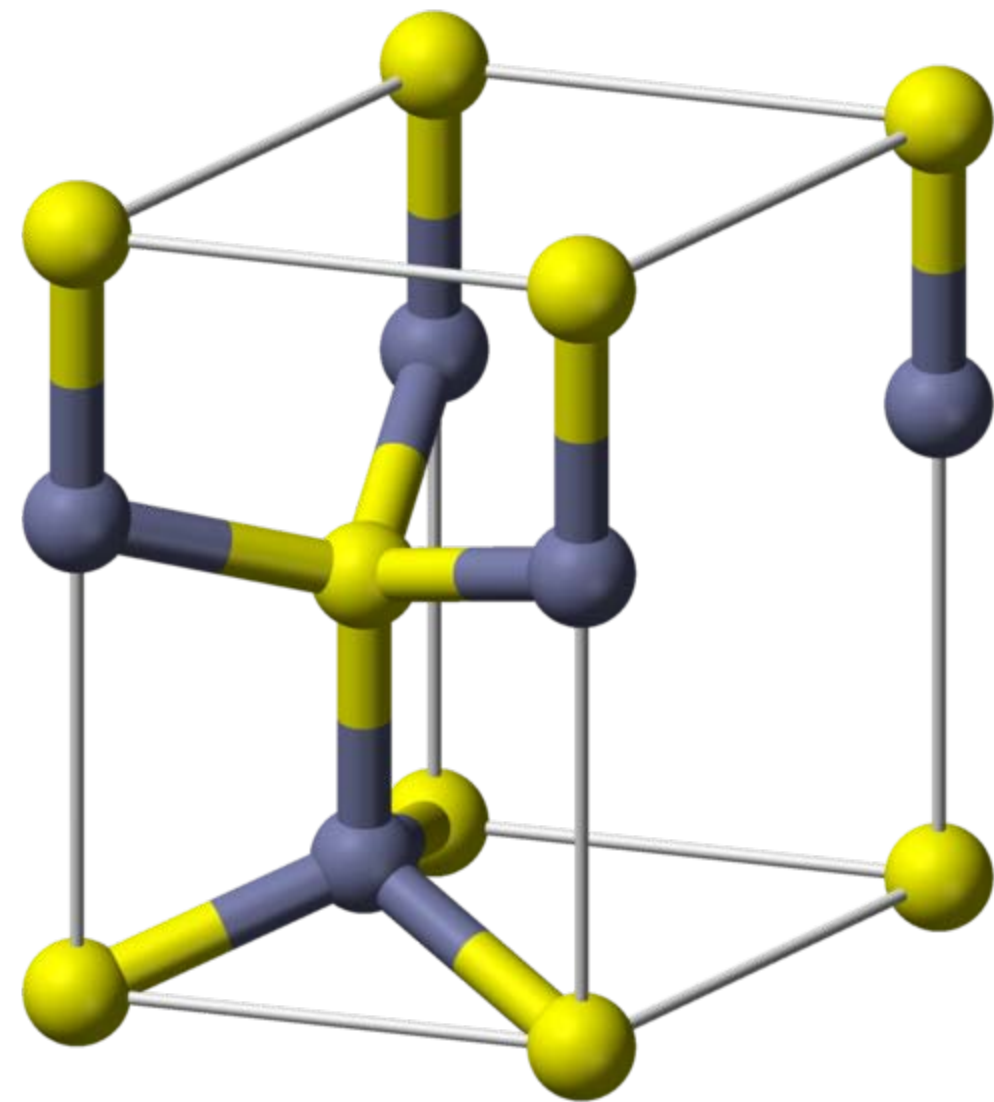


Tetrahedral
coordination

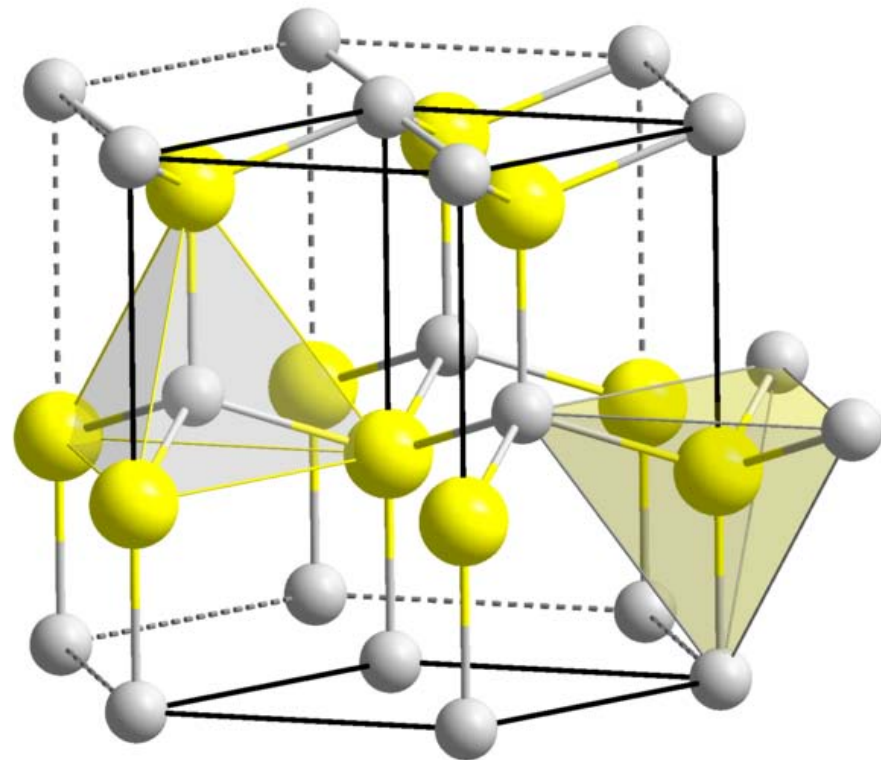


ZnS or zinc blende

$F\bar{4}3m$

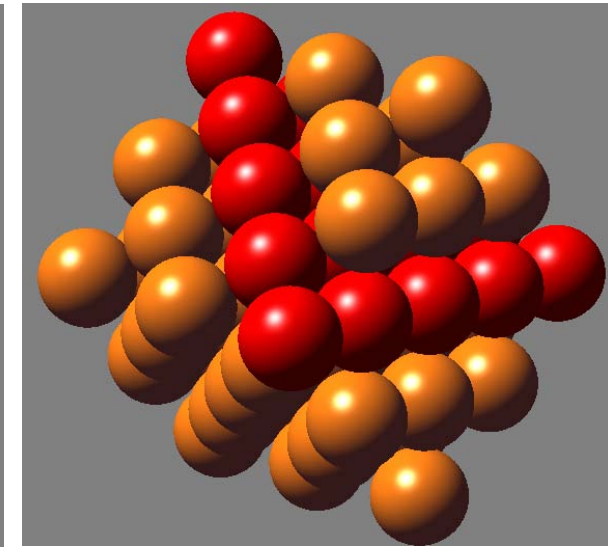
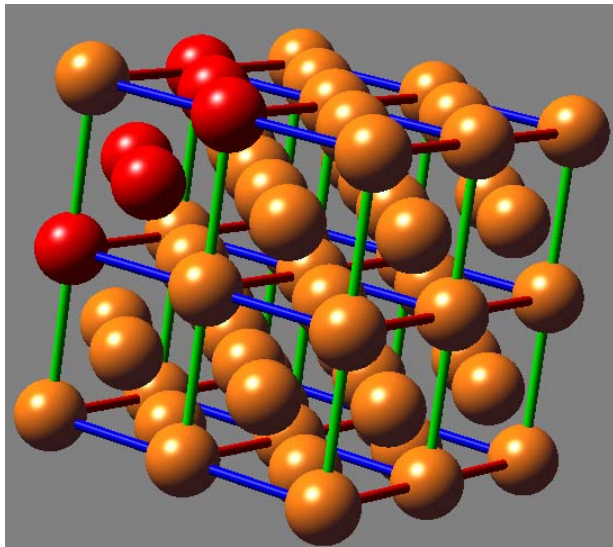
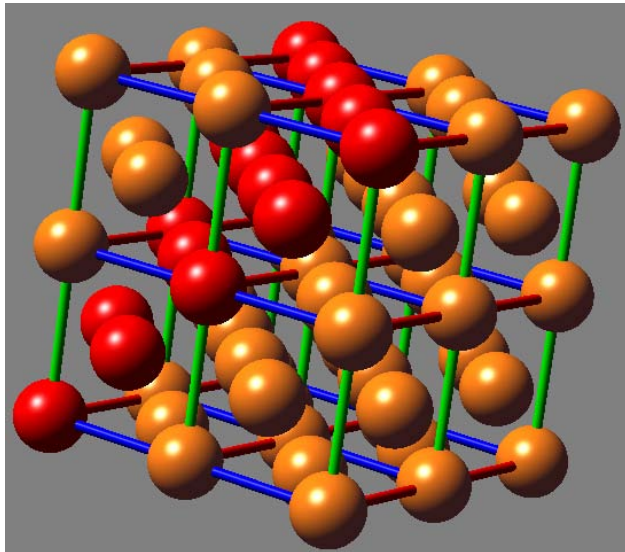
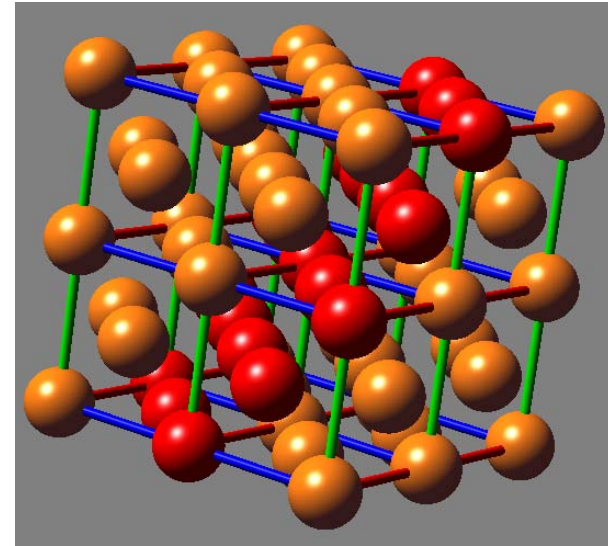
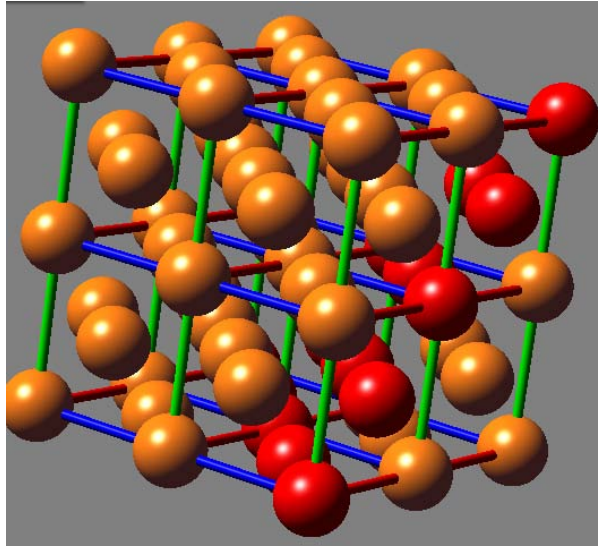
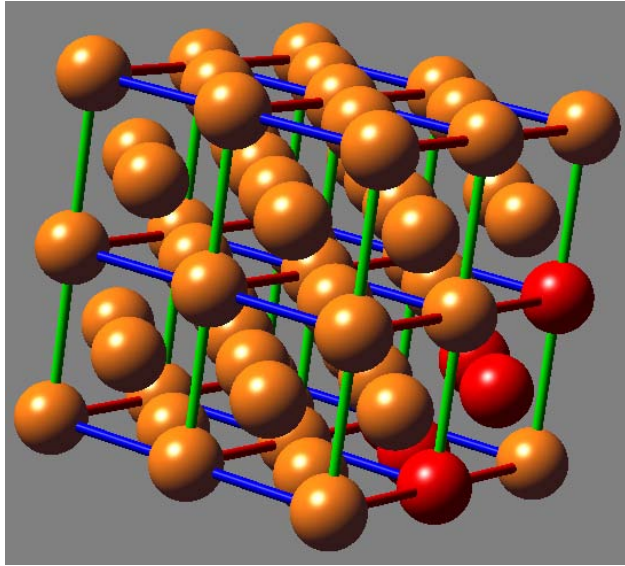


wurtzite

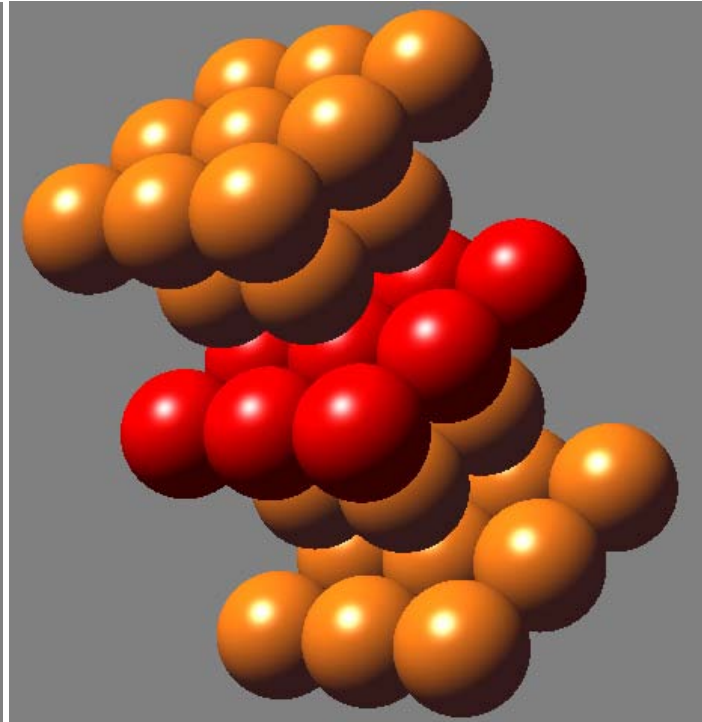
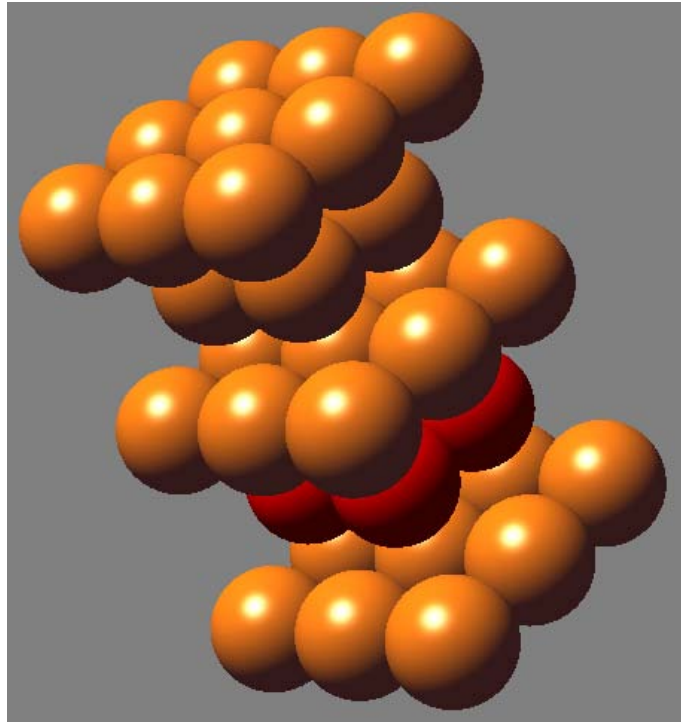
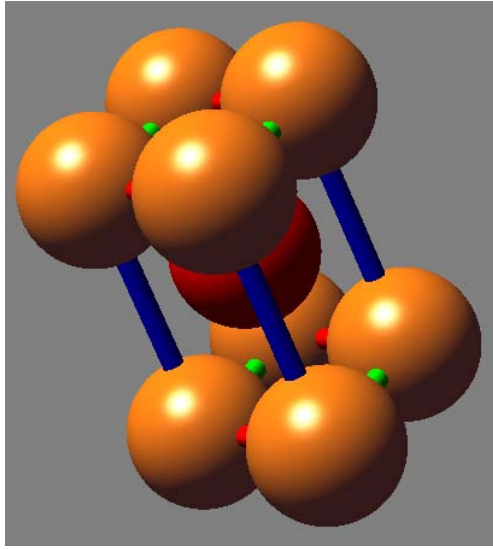


$P6_3mc$

Face-centred close packing (f.c.p.)



$\overline{Fm3m}$



hexagonal close
packing (h.c.p.)

$P6_3 / mmc$

