

from Wyckoff to Quantum ESPRESSO

How to translate a crystallographic structure as given in standard texts (ex. Ralph W.G. Wyckoff, *Crystal Structures*) into the Quantum ESPRESSO input format.

How is a crystal structure defined in QE ?

The **&SYSTEM** namelist (STRUCTURE)

ibrav Bravais-lattice index (NO default, must be specified)

0	read unit cell information from CELL_PARAMETERS card
1	cubic P (sc)
2	cubic F (fcc)
3	cubic I (bcc)
4	Hexagonal and Trigonal P
5	Trigonal R
6	Tetragonal P (st)
7	Tetragonal I (bct)
8	Orthorhombic P
9	Orthorhombic base-centered(bco)
10	Orthorhombic face-centered
11	Orthorhombic body-centered
12	Monoclinic P
13	Monoclinic base-centered
14	Triclinic P

The **&SYSTEM** namelist (STRUCTURE) continued

Crystallographic constants: there are two options

- 1) `celldm(i)`, $i=1,2,\dots,6$
- 2) `a`, `b`, `c`, `cosab`, `cosac`, `cosbc`,

```
celldm(1) = a / bohr_radius_angs = alat (internal unit of length)
celldm(2) = b / a
celldm(3) = c / a
celldm(4) = cosab
celldm(5) = cosac
celldm(6) = cosbc
```

BEWARE:

`alat = celldm(1)` is the lattice parameter "a" in BOHR
`a,b,c` are given in ANGSTROM

Specify either `a,b,c,...` , **OR** `celldm` **but not both**. Only crystallographic constants needed for chosen Bravais lattice must be specified; other parameters are **IGNORED**.

The &SYSTEM namelist (STRUCTURE) continued

		a	b	c	cosab	cosac	cosbc
ibrav	celldm -->	1	2	3	4	5	6
1 cubic P (sc)		*					
2 cubic F (fcc)		*					
3 cubic I (bcc)		*					
4 Hexagonal and Trigonal P		*		*			
5 Trigonal R		*			*		
6 Tetragonal P (st)		*		*			
7 Tetragonal I (bct)		*		*			
8 Orthorhombic P		*	*	*			
9 Orthorhombic base-centered(bco)		*	*	*			
10 Orthorhombic face-centered		*	*	*			
11 Orthorhombic body-centered		*	*	*			
12 Monoclinic P		*	*	*	*		
13 Monoclinic base-centered		*	*	*	*		
14 Triclinic P		*	*	*	*	*	*

The **&SYSTEM** namelist (STRUCTURE) continued

If **ibrav = 0** BL fundamental vectors are read from an optional card **CELL_PARAMETERS** to be inserted after all needed NAMELISTS.

```
&LAST_REQUIRED_NAMELIST
```

```
...
```

```
/
```

```
CELL_PARAMETERS    symmetry_class
```

```
  a(1,1) a(2,1) a(3,1)
```

```
  a(1,2) a(2,2) a(3,2)
```

```
  a(1,3) a(2,3) a(3,3)
```

Where **symmetry_class** is **cubic** or **hexagonal** depending on the expected symmetry of the system w.r.t. the **assumed** reference system.

If **celldm(1)≠0**, lattice vectors are given in **these units**

If **celldm(1)=0**, lattice vectors are given in **BOHR**, and the length of the first lattice vector defines **alat**.

The &SYSTEM namelist (STRUCTURE) continued

nat INTEGER (NO default, must be specified)
 number of atoms in the unit cell

ntyp INTEGER (NO default, must be specified)
 number of types of atoms in the unit cell

nelec REAL
 number of electron in the unit cell
 Default: the same as ionic charge (neutral cell)

nbnd INTEGER
 number of electronic bands to be calculated.
 Default: in insulators, $\text{nbnd} = \text{nelec}/2$
 in metals, 20% more (minimum 4 more)

The `ATOMIC_SPECIES` card

For each atomic species (`ntyp` in `&SYSTEM` namelist) one must specify a label, the atomic mass and the name a PP file.

```
ATOMIC_SPECIES
```

```
X(1)      Mass_X(1)      PseudoPot_X(1)
```

```
...
```

```
X(ntyp)  Mass_X(ntyp)  PseudoPot_X(ntyp)
```


The `ATOMIC_SPECIES` card

For each atomic species (`ntyp` in `&SYSTEM` namelist) one must specify a label, the atomic mass and the name a PP file.

```
ATOMIC_SPECIES
```

```
X(1)      Mass_X(1)      PseudoPot_X(1)
```

```
...
```

```
X(ntyp) Mass_X(ntyp)  PseudoPot_X(ntyp)
```

example

```
ATOMIC_SPECIES
```

```
O  16.00  O.LDA.US.RRKJ3.UPF
```

```
C   12.00  C.pz-rrkjus.UPF
```

The **ATOMIC_SPECIES** card

For each atomic species (ntyp in &SYSTEM namelist) one must specify a **label**, the **atomic mass** and the **name a PP file**.

```
ATOMIC_SPECIES
```

```
X(1)      Mass_X(1)      PseudoPot_X(1)
```

```
...
```

```
X(ntyp) Mass_X(ntyp) PseudoPot_X(ntyp)
```

example

```
ATOMIC_SPECIES
```

```
O  16.00  O.LDA.US.RRKJ3.UPF
```

```
C   12.00  C.pz-rrkjus.UPF
```

Masses are actually used only if atoms move.

The **ATOMIC_POSITIONS** card

This card specifies the atomic species **label** and **positions** of each atom in the unit cell (nat in &SYSTEM namelist).

```
ATOMIC_POSITIONS  position_format  
X(1)    x(1)    y(1)    z(1)  
...  
X(nat)  x(nat)  y(nat)  z(nat)
```

where **position_format** is **alat** (default), **bohr**, **angstrom** or **crystal**

The `ATOMIC_POSITIONS` card

This card specifies the atomic species `label` and `positions` of each atom in the unit cell (nat in `&SYSTEM` namelist).

```
ATOMIC_POSITIONS position_format
X(1)    x(1)    y(1)    z(1)
...
X(nat)  x(nat)  y(nat)  z(nat)
```

where `position_format` is `alat` (default), `bohr`, `angstrom` or `crystal`.
It is also possible to specify that some coordinates should be kept fixed in relaxation or dynamics.

```
ATOMIC_POSITIONS bohr
C 2.256 0.0 0.0
O 0.0 0.0 0.0 0 0 0
```

A few examples

diamond

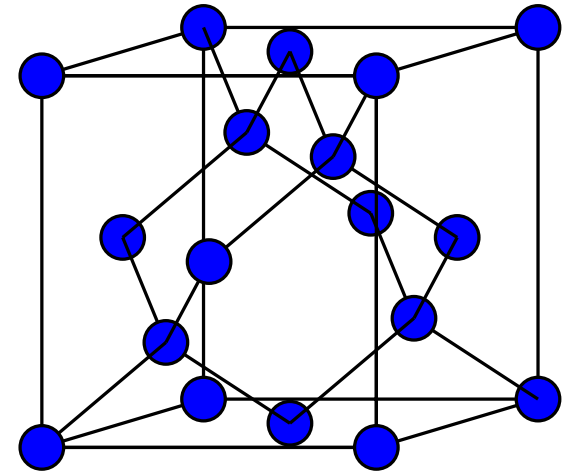
II,i1: The unit cubes of crystals with the *diamond structure* have eight atoms in the position of O_h^7 ($Fd3m$):

$$(8a) \quad 000; 0 \quad 1/2 \quad 1/2; \quad 1/2 \quad 0 \quad 1/2; \quad 1/2 \quad 1/2 \quad 0; \\ 1/4 \quad 1/4 \quad 1/4; \quad 1/4 \quad 3/4 \quad 3/4; \quad 3/4 \quad 1/4 \quad 3/4; \quad 3/4 \quad 3/4 \quad 1/4$$

or more briefly

$$(8a) \quad 000; \quad 1/4 \quad 1/4 \quad 1/4; \quad \text{F.C.}$$

Element	Name	a_0 , Å
C	carbon	3.56679 (20 C)
Si	Silicon	5.43070 (25 C) 5.445 (1300 C)
Ge	Germanium	5.65735 (20 C) 5.65695 (18 C)
α -Sn	Tin (gray)	6.4912



diamond

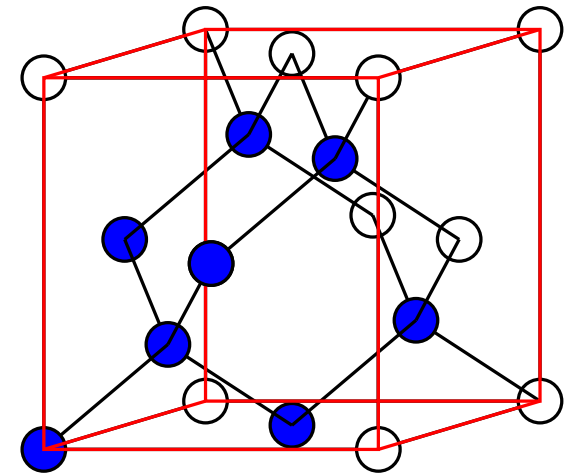
II,i1: The unit cubes of crystals with the *diamond structure* have eight atoms in the position of O_h^7 ($Fd3m$):

$$(8a) \quad 000; 0 \quad 1/2 \quad 1/2; \quad 1/2 \quad 0 \quad 1/2; \quad 1/2 \quad 1/2 \quad 0; \\ 1/4 \quad 1/4 \quad 1/4; \quad 1/4 \quad 3/4 \quad 3/4; \quad 3/4 \quad 1/4 \quad 3/4; \quad 3/4 \quad 3/4 \quad 1/4$$

or more briefly

$$(8a) \quad 000; \quad 1/4 \quad 1/4 \quad 1/4; \quad \text{F.C.}$$

Element	Name	a_0 , Å
C	carbon	3.56679 (20 C)
Si	Silicon	5.43070 (25 C) 5.445 (1300 C)
Ge	Germanium	5.65735 (20 C) 5.65695 (18 C)
α -Sn	Tin (gray)	6.4912



C: simple cubic \longrightarrow ibrav = 1
3.56679 A

&SYSTEM

ntyp=1, nat=8, ibrav=1, a = 3.56679,

/

...

ATOMIC_SPECIES

C 28.086 C.UPF

ATOMIC_POSITIONS

C 0.0 0.0 0.0

C 0.0 0.5 0.5

C 0.5 0.0 0.5

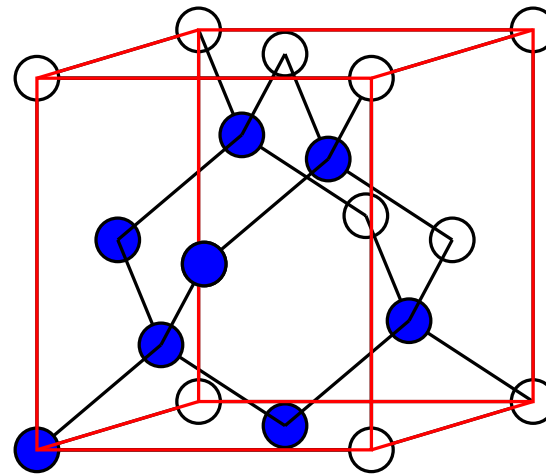
C 0.5 0.5 0.0

C 0.25 0.25 0.25

C 0.25 0.75 0.75

C 0.75 0.25 0.75

C 0.75 0.75 0.25



C: simple cubic \longrightarrow ibrav = 1
3.56679 Å \longrightarrow 6.740259 bohrs

&SYSTEM

ntyp=1, nat=8, ibrav=1, celldm(1)=6.740259,

/

...

ATOMIC_SPECIES

C 28.086 C.UPF

ATOMIC_POSITIONS

C 0.0 0.0 0.0

C 0.0 0.5 0.5

C 0.5 0.0 0.5

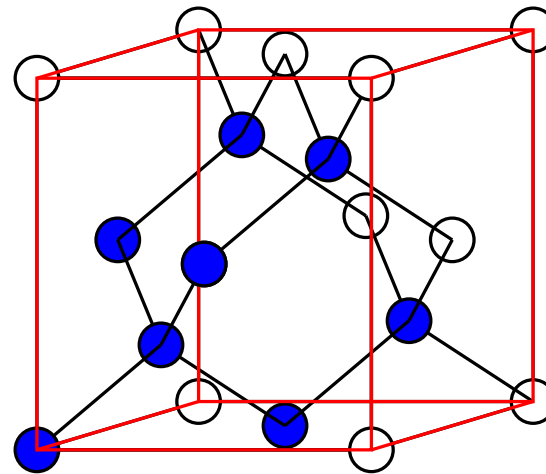
C 0.5 0.5 0.0

C 0.25 0.25 0.25

C 0.25 0.75 0.75

C 0.75 0.25 0.75

C 0.75 0.75 0.25



C: simple cubic \longrightarrow ibrav = 1
3.56679 Å \longrightarrow 6.740259 bohrs

&SYSTEM

ntyp=1, nat=8, ibrav=1, celldm(1)=6.740259,

/

...

ATOMIC_SPECIES

C 28.086 C.UPF

ATOMIC_POSITIONS

C 0.0 0.0 0.0

C 0.0 0.5 0.5

C 0.5 0.0 0.5

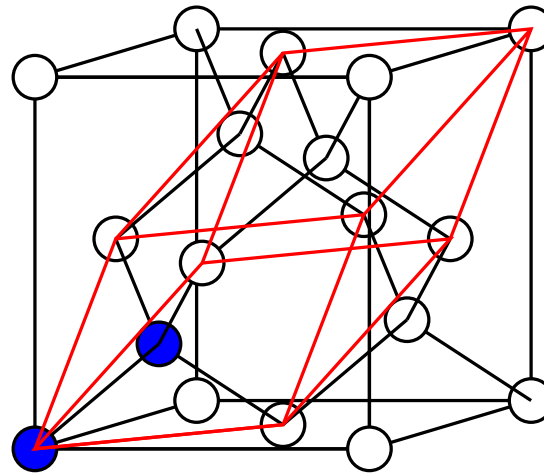
C 0.5 0.5 0.0

C 0.25 0.25 0.25

C 0.25 0.75 0.75

C 0.75 0.25 0.75

C 0.75 0.75 0.25



C: face centered cubic \longrightarrow ibrav = 2
3.56679 Å \longrightarrow 6.740259 bohrs

&SYSTEM

ntyp=1, nat=2, ibrav=2, celldm(1)=6.740259,

/

...

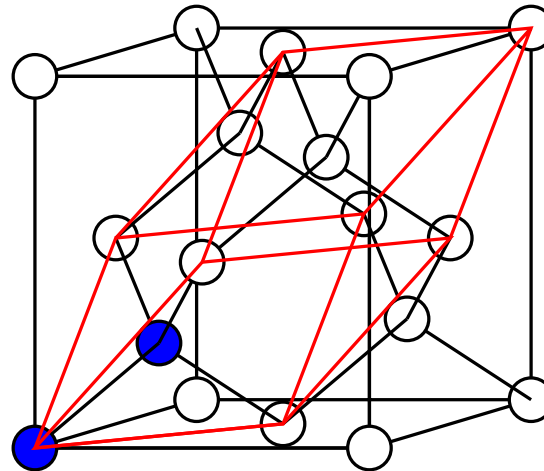
ATOMIC_SPECIES

C 28.086 C.UPF

ATOMIC_POSITIONS

C 0.0 0.0 0.0

C 0.25 0.25 0.25

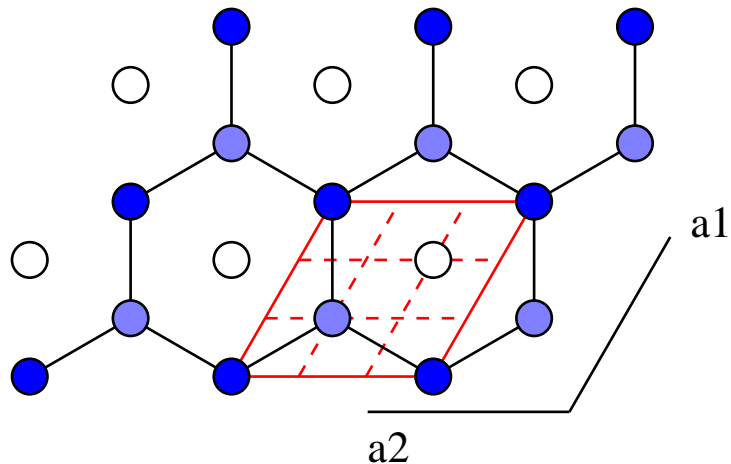
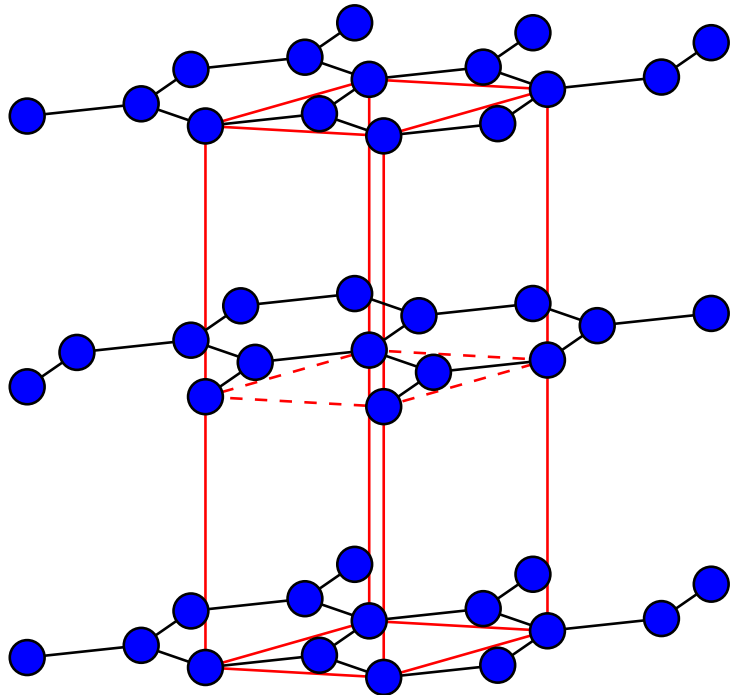


graphite

II,i2: The long-familiar form of *graphite* has an hexagonal unit with
 $a_0 = 2.456 \text{ \AA}$, $c_0 = 6.696 \text{ \AA}$

Its four atoms are in the following two sets of special positions of C_{6v}^4
($C6mc$):

(2a) $00u$; $0,0,u+1/2$ and (2b) $1/3 \ 2/3 \ v$; $2/3, 1/3, v + 1/2$
where u can be taken as zero; v then is practically zero and cannot
exceed 0.05

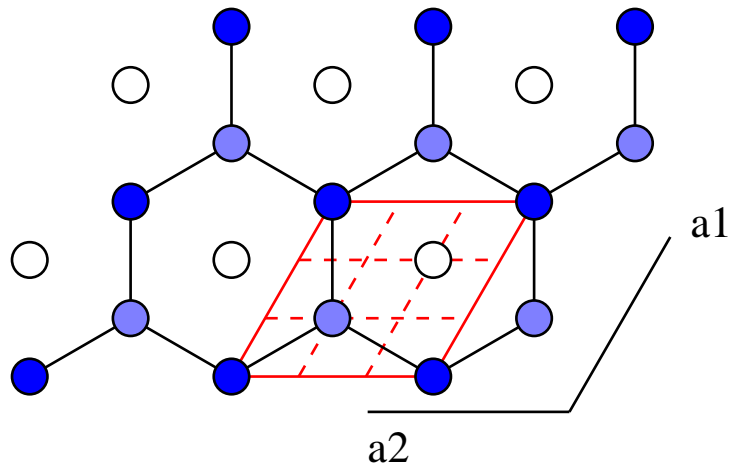
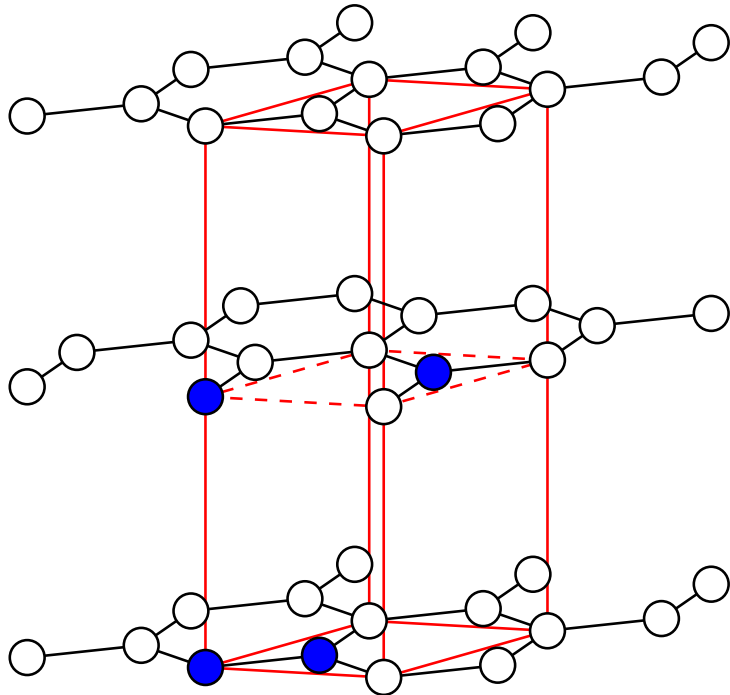


graphite

II,i2: The long-familiar form of *graphite* has an hexagonal unit with
 $a_0 = 2.456 \text{ \AA}$, $c_0 = 6.696 \text{ \AA}$

Its four atoms are in the following two sets of special positions of C_{6v}^4
($C6mc$):

(2a) $00u$; $0,0,u+1/2$ and (2b) $1/3 \ 2/3 \ v$; $2/3, 1/3, v + 1/2$
where u can be taken as zero; v then is practically zero and cannot
exceed 0.05



hexagonal \longrightarrow ibrav = 4
a = 2.456 Å, c = 6.696 Å
u = v = 0

&SYSTEM

ibrav=4, a = 2.456, c = 6.696,
ntyp=1, nat=4,

/

...

ATOMIC_SPECIES

C 28.086 C.UPF

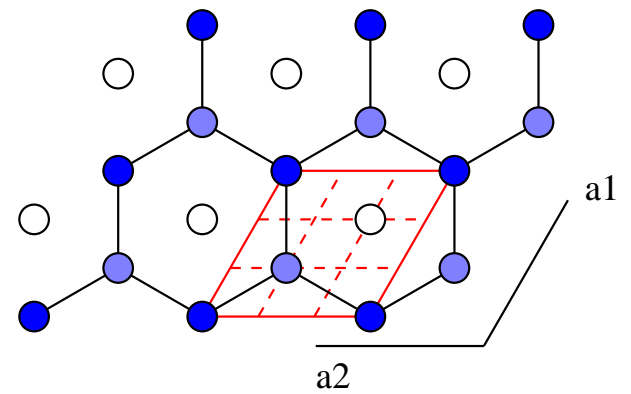
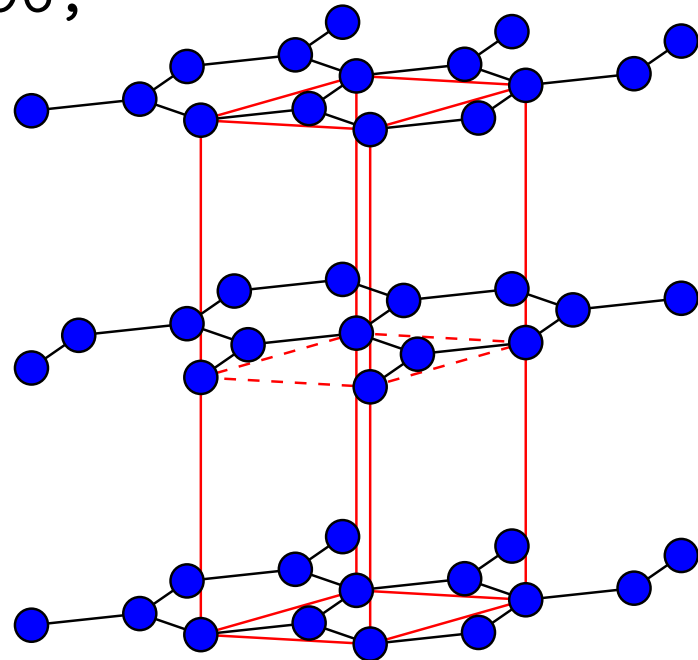
ATOMIC_POSITIONS crystal

C 0.0 0.0 0.0

C 0.3333333333 0.6666666666 0.0

C 0.0 0.0 0.5

C 0.6666666666 0.3333333333 0.5



hexagonal \longrightarrow ibrav = 4

$a = 2.456 \text{ \AA}$, $c = 6.696 \text{ \AA}$ \longrightarrow $a = 4.64117 \text{ bohrs}$, $c/a = 2.7264$

$u = v = 0$

&SYSTEM

ibrav=4, celldm(1)=4.64117, celldm(3)= 2.7264,

ntyp=1, nat=4,

/

...

ATOMIC_SPECIES

C 28.086 C.UPF

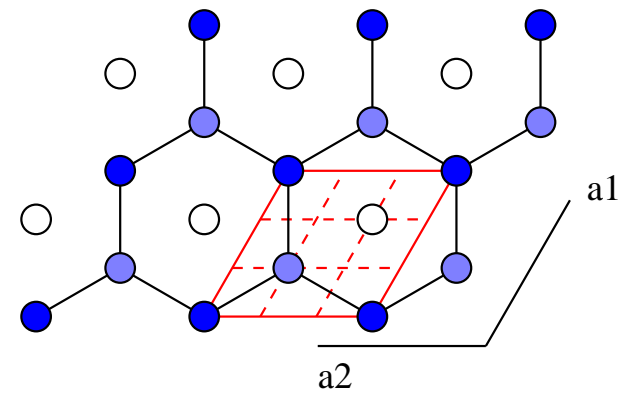
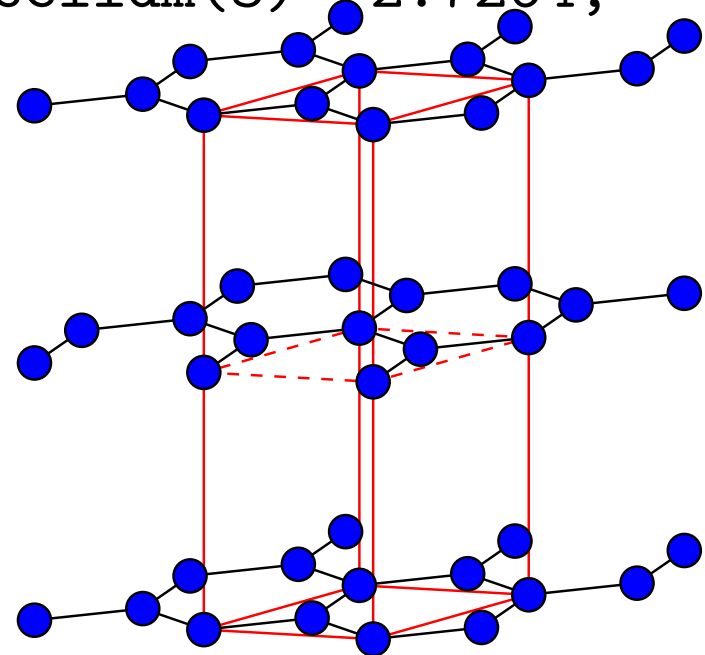
ATOMIC_POSITIONS crystal

C 0.0 0.0 0.0

C 0.3333333333 0.6666666666 0.0

C 0.0 0.0 0.5

C 0.6666666666 0.3333333333 0.5



hexagonal \longrightarrow ibrav = 4

$a = 2.456 \text{ \AA}$, $c = 6.696 \text{ \AA} \longrightarrow a = 4.64117 \text{ bohrs}$, $c/a = 2.7264$

$u = v = 0$

$0.5 \text{ } c/a = 1.3632$

&SYSTEM

ibrav=4, celldm(1)=4.64117, celldm(3)= 2.7264,

ntyp=1, nat=4,

/

...

ATOMIC_SPECIES

C 28.086 C.UPF

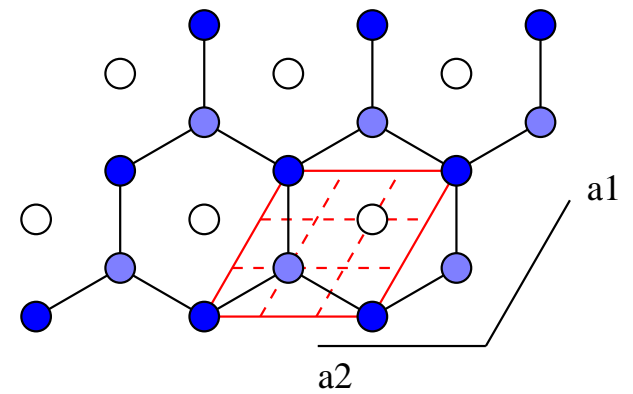
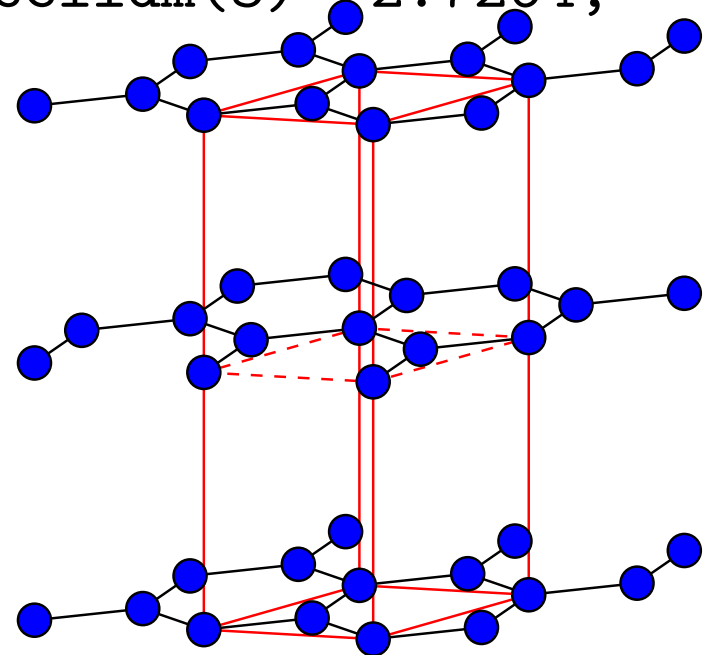
ATOMIC_POSITIONS

C 0.0 0.0 0.0

C 0.0 0.57735027 0.0

C 0.0 0.0 1.3632

C 0.5 0.28867513 1.3632



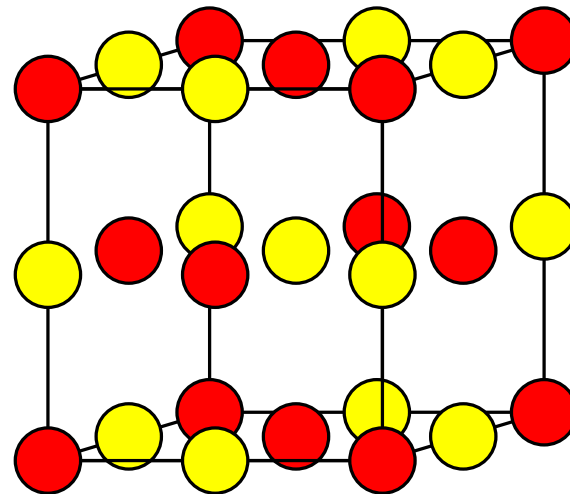
sodium chloride

III, a1: The largest group of RX-type crystals have the structure of *sodium chloride*, NaCl. The unit cube of this arrangement contains four molecules with atoms in the positions:

R: (4a) 000; $1/2\ 1/2\ 0$; $1/2\ 0\ 1/2$; $0\ 1/2\ 1/2$, or 000; FC

X: (4b) $1/2\ 1/2\ 1/2$; $1/2\ 0\ 0$; $0\ 1/2\ 0$; $0\ 0\ 1/2$, or $1/2\ 1/2\ 1/2$; FC

Crystal	a_0 A
....	
MgO	4.21112 (21 C)
....	
NaCl	5.62779 (18 C)
....	
NiO	4.1684
....	



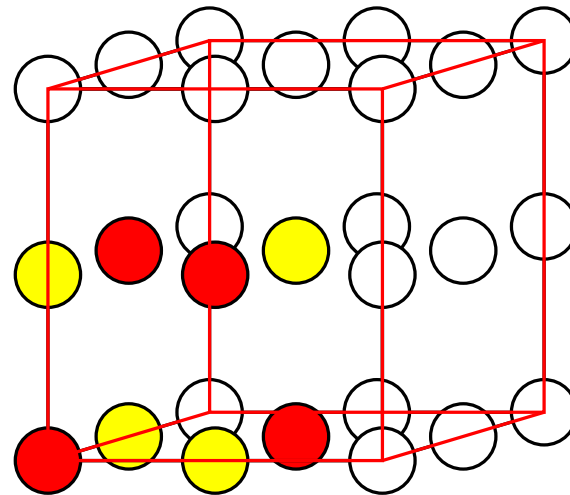
sodium chloride

III, a1: The largest group of RX-type crystals have the structure of *sodium chloride*, NaCl. The unit cube of this arrangement contains four molecules with atoms in the positions:

R: (4a) 000; $1/2\ 1/2\ 0$; $1/2\ 0\ 1/2$; $0\ 1/2\ 1/2$, or 000; FC

X: (4b) $1/2\ 1/2\ 1/2$; $1/2\ 0\ 0$; $0\ 1/2\ 0$; $0\ 0\ 1/2$, or $1/2\ 1/2\ 1/2$; FC

Crystal	a_0 A
....	
MgO	4.21112 (21 C)
....	
NaCl	5.62779 (18 C)
....	
NiO	4.1684
....	



MgO: face centered cubic \longrightarrow ibrav = 2
4.21112 Å \longrightarrow 7.957867 bohrs

&SYSTEM

ntyp=2, nat=2, ibrav=2, celldm(1)=7.957867,

/

...

ATOMIC_SPECIES

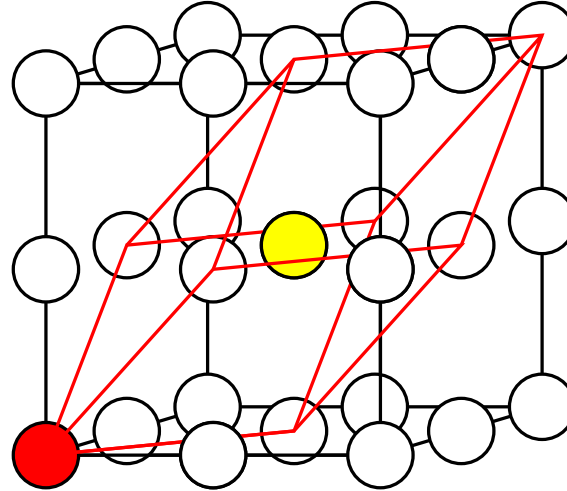
Mg 28.086 Mg.UPF

O 16.000 O.UPF

ATOMIC_POSITIONS

Mg 0.0 0.0 0.0

O 0.5 0.5 0.5



NiO: face centered cubic \longrightarrow ibrav = 2
4.1684 Å \longrightarrow 7.87714 bohrs

&SYSTEM

ntyp=2, nat=2, ibrav=2, celldm(1)= 7.87714,

/

...

ATOMIC_SPECIES

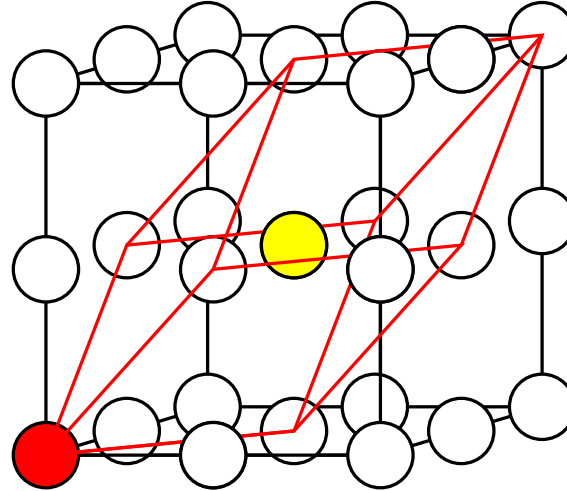
Ni 28.086 Ni.UPF

O 16.000 O.UPF

ATOMIC_POSITIONS

Ni 0.0 0.0 0.0

O 0.5 0.5 0.5



NiO: face centered cubic \longrightarrow ibrav = 2
4.1684 Å \longrightarrow 7.87714 bohrs

&SYSTEM

ntyp=2, nat=2, ibrav=2, celldm(1)= 7.87714,

/

...

ATOMIC_SPECIES

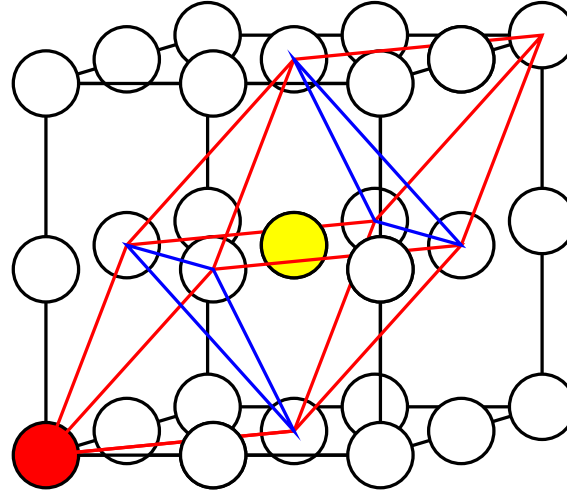
Ni 28.086 Ni.UPF

O 16.000 O.UPF

ATOMIC_POSITIONS

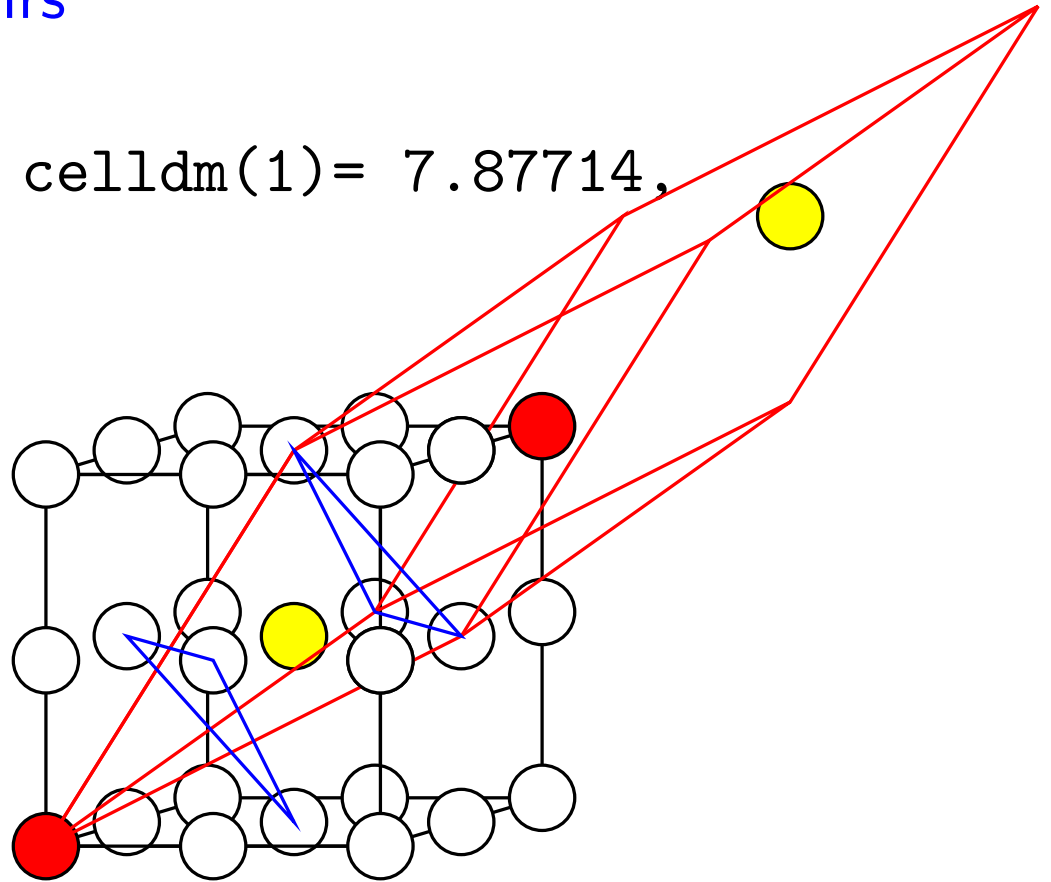
Ni 0.0 0.0 0.0

O 0.5 0.5 0.5



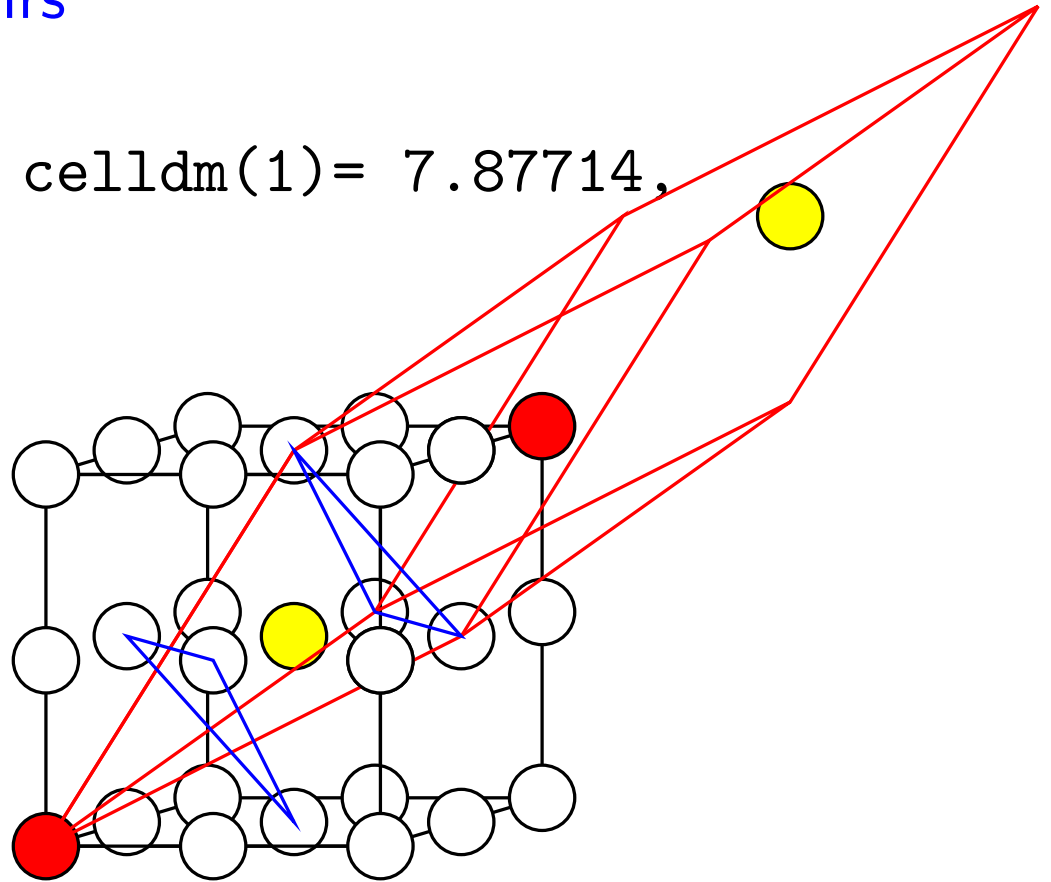
NiO: face centered cubic \longrightarrow ibrav = 2
4.1684 Å \longrightarrow 7.87714 bohrs

```
&SYSTEM
  ntyp=2, nat=2, ibrav=2, celldm(1)= 7.87714,
/
...
ATOMIC_SPECIES
Ni 28.086 Ni.UPF
O  16.000 O.UPF
ATOMIC_POSITIONS
Ni 0.0 0.0 0.0
O  0.5 0.5 0.5
```



NiO: user supplied lattice \longrightarrow ibrav = 0
4.1684 Å \longrightarrow 7.87714 bohrs

```
&SYSTEM
  ntyp=3, nat=4, ibrav=0, celldm(1)= 7.87714,
/
CELL_PARAMETERS cubic
1.00 0.50 0.50
0.50 1.00 0.50
0.50 0.50 1.00
ATOMIC_SPECIES
Ni1 1. Ni.UPF
Ni2 1. Ni.UPF
O 1. O.UPF
ATOMIC_POSITIONS crystal
Ni1 0.0 0.0 0.0
Ni2 0.5 0.5 0.5
O 0.25 0.25 0.25
O 0.75 0.75 0.75
```



NiO: rhombohedral lattice \longrightarrow ibrav = 5

$$4.1684 \text{ \AA} \times \sqrt{3/2} = 5.1052265 \text{ \AA}, \cos(ab)=5/6$$

&SYSTEM

ntyp=3, nat=4, ibrav=5,

a = 5.1052265, cosab = 0.83333333,

/

ATOMIC_SPECIES

Ni1 1. Ni.UPF

Ni2 1. Ni.UPF

O 1. O.UPF

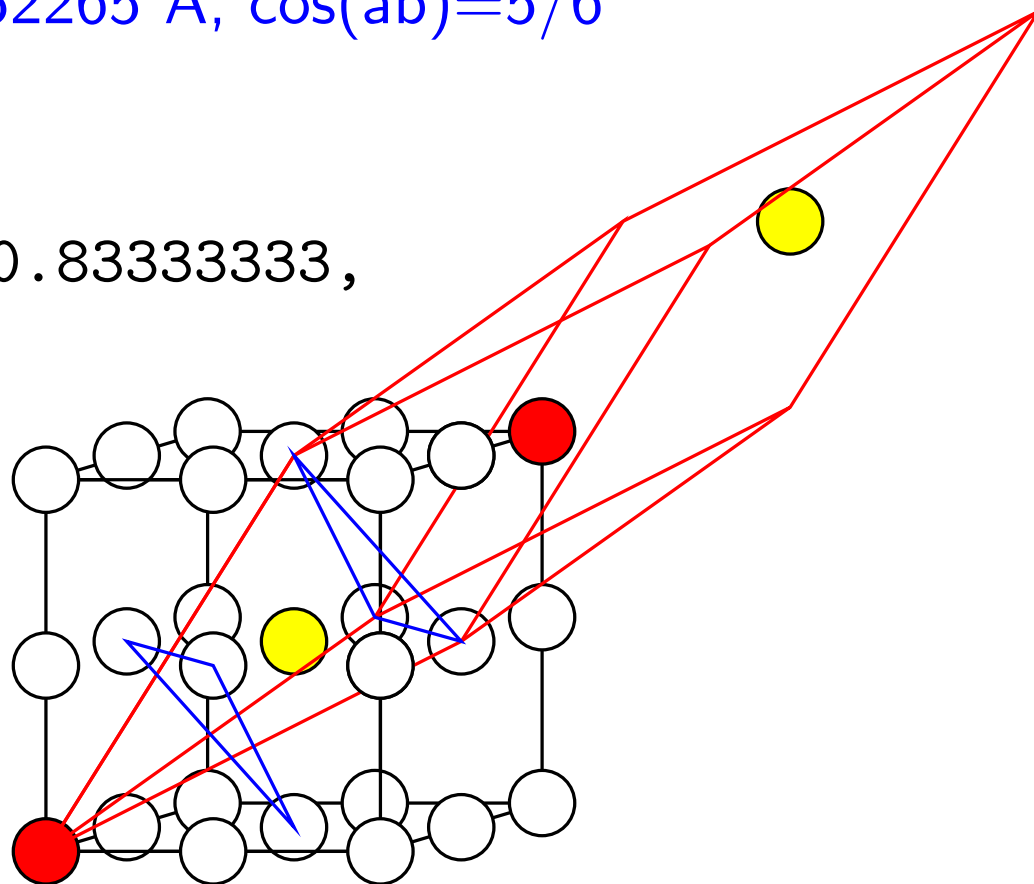
ATOMIC_POSITIONS crystal

Ni1 0.0 0.0 0.0

Ni2 0.5 0.5 0.5

O 0.25 0.25 0.25

O 0.75 0.75 0.75



NiO: rhombohedral lattice \longrightarrow ibrav = 5

$$4.1684 \text{ \AA} \times \sqrt{3/2} = 9.64748375 \text{ bohrs, } \cos(ab)=5/6$$

&SYSTEM

ntyp=3, nat=4, ibrav=5,

celldm(1) =9.64748375, celldm(4) = 0.83333333,

/

ATOMIC_SPECIES

Ni1 1. Ni.UPF

Ni2 1. Ni.UPF

O 1. O.UPF

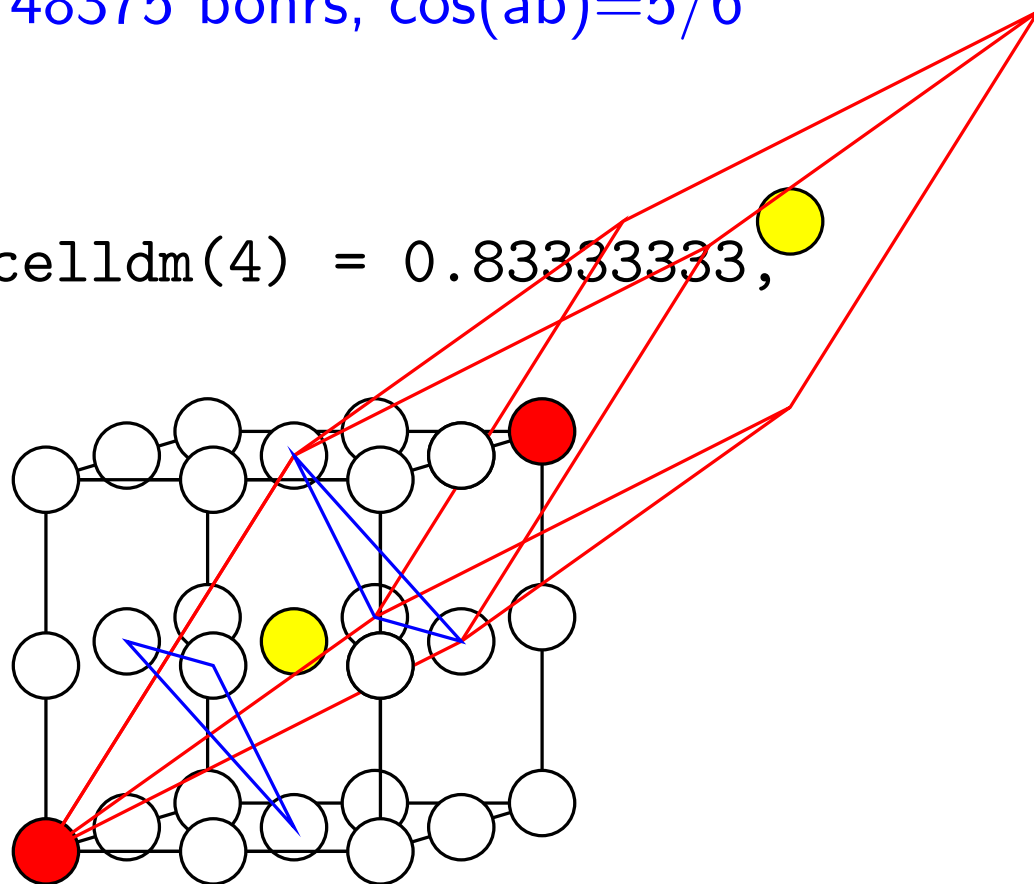
ATOMIC_POSITIONS crystal

Ni1 0.0 0.0 0.0

Ni2 0.5 0.5 0.5

O 0.25 0.25 0.25

O 0.75 0.75 0.75



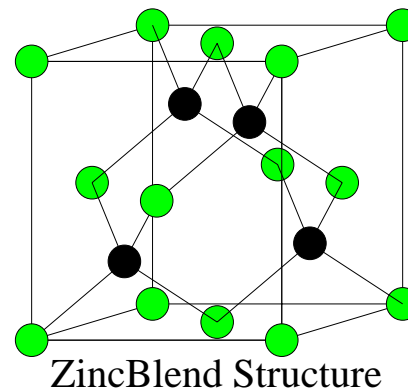
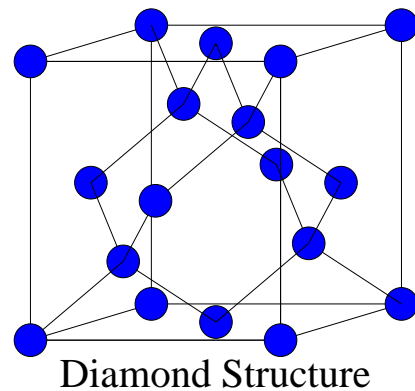
zinc-blend

III, c1: The *zinc sulfide* arrangement, like that of NaCl contains four molecules in its unit cube and is developed on a face-centered lattice. Its atoms have the coordinates (of $T_d^2 - F\bar{4}3m$):

R: (4a) 000; $1/2\ 1/2\ 0$; $1/2\ 0\ 1/2$; $0\ 1/2\ 1/2$, or 000; FC

X: (4c) $1/4\ 1/4\ 1/4$; $1/4\ 3/4\ 3/4$; $3/4\ 1/4\ 3/4$; $3/4\ 3/4\ 1/4$, or $1/4\ 1/4\ 1/4$; F.C.

As can be seen each atom has about it four equally distant atoms of the opposite sort arranged at the corners of a regular tetrahedron. If all atoms were alike this would, of course, be the diamond arrangement (II,i1).



ZnS: face centered cubic \longrightarrow ibrav = 2
5.65 \longrightarrow 10.68 bohrs

&SYSTEM

ntyp=2, nat=2, ibrav=2, celldm(1)=10.68,

/

...

ATOMIC_SPECIES

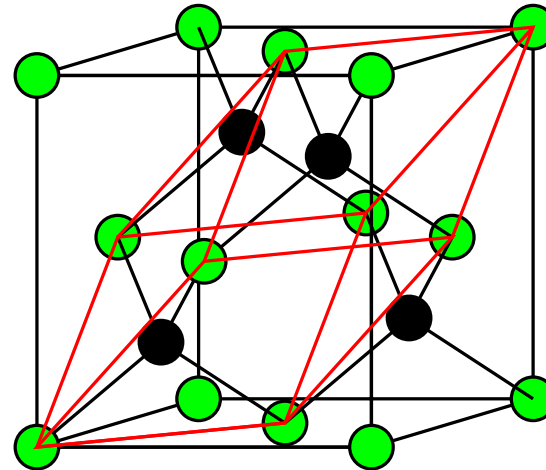
Zn 1. Zn.UPF

S 1. S.UPF

ATOMIC_POSITIONS

Zn 0.0 0.0 0.0

S 0.25 0.25 0.25



ZnS: face centered cubic \longrightarrow ibrav = 2
5.65 \longrightarrow 10.68 bohrs

&SYSTEM

ntyp=2, nat=2, ibrav=2, celldm(1)=10.68,

/

...

ATOMIC_SPECIES

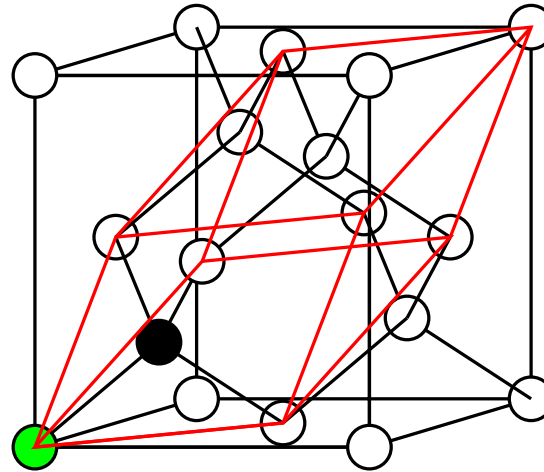
Zn 1. Zn.UPF

S 1. S.UPF

ATOMIC_POSITIONS

Zn 0.0 0.0 0.0

S 0.25 0.25 0.25



wurtzite

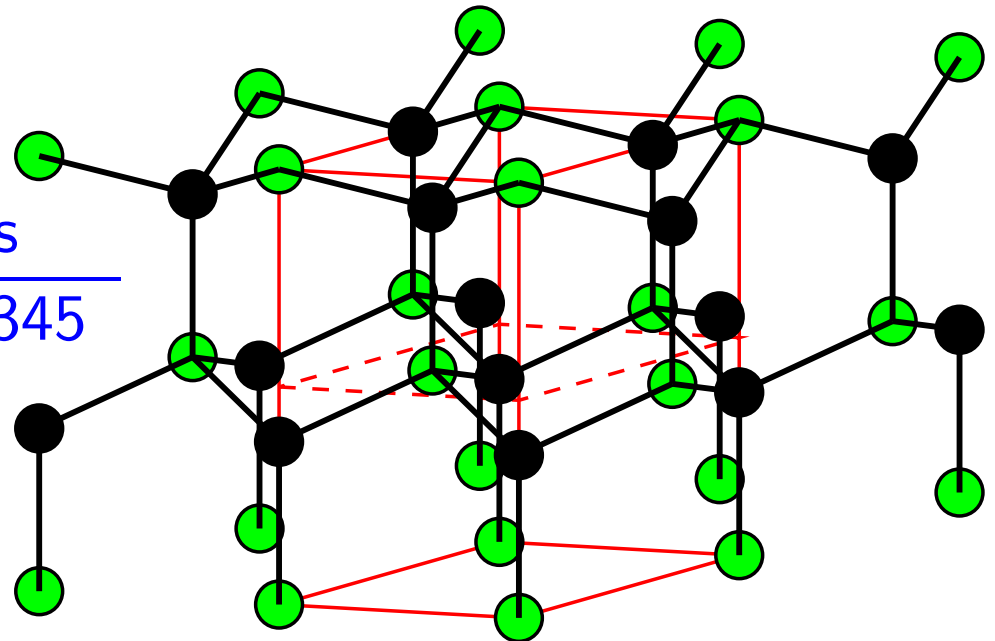
III,c1: The atoms in the two-molecule hexagonal unit of the *zincite*, ZnO, arrangement are in the positions:

R: 000. $1/3$ $2/3$ $1/2$

X: $00u$, $1/3$ $2/3$ $u+1/2$

The axial ratio of crystals with this structure have always been close to $c/a=1.63$, and the parameter u to 0.375. Under this circumstances each atom has about it a tetrahedron of atoms of the opposite sort just as in the cubic ZnS arrangement.

Crystal	a_0	c_0	remarks
ZnO	3.24950	5.2069	$u = 0.345$
ZnS	3.811	6.234	



ZnO: hexagonal \longrightarrow ibrav = 4

$a = 3.24950$ A, $c = 5.2069$ A $\longrightarrow c/a=1.60236959$

$u = 0.345$

&SYSTEM

ntyp=2, nat=4, ibrav=4, a = 3.24950, c = 5.2069,

/

...

ATOMIC_SPECIES

Zn 1. Zn.UPF

O 1. O.UPF

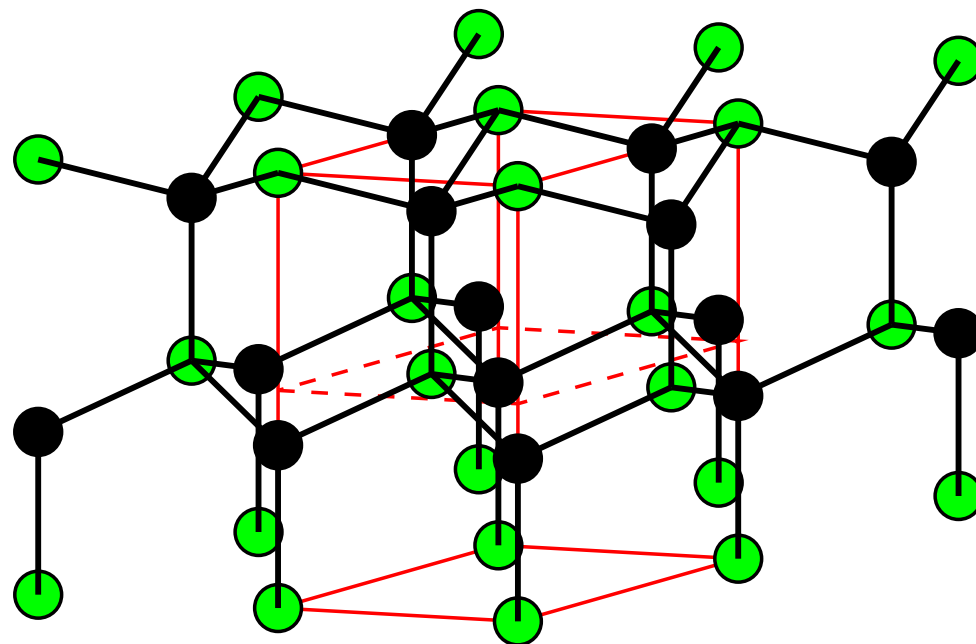
ATOMIC_POSITIONS crystal

Zn 0.0 0.0 0.0

Zn 0.33333333 0.66666666 0.5

O 0.0 0.0 0.345

O 0.66666666 0.33333333 0.845



ZnO: hexagonal \longrightarrow ibrav = 4

$a = 3.24950$ A, $c = 5.2069$ A $\longrightarrow c/a=1.60236959$

$u = 0.345$

&SYSTEM

ntyp=2, nat=4, ibrav=4, a = 3.24950, c = 5.2069,

/

...

ATOMIC_SPECIES

Zn 1. Zn.UPF

O 1. O.UPF

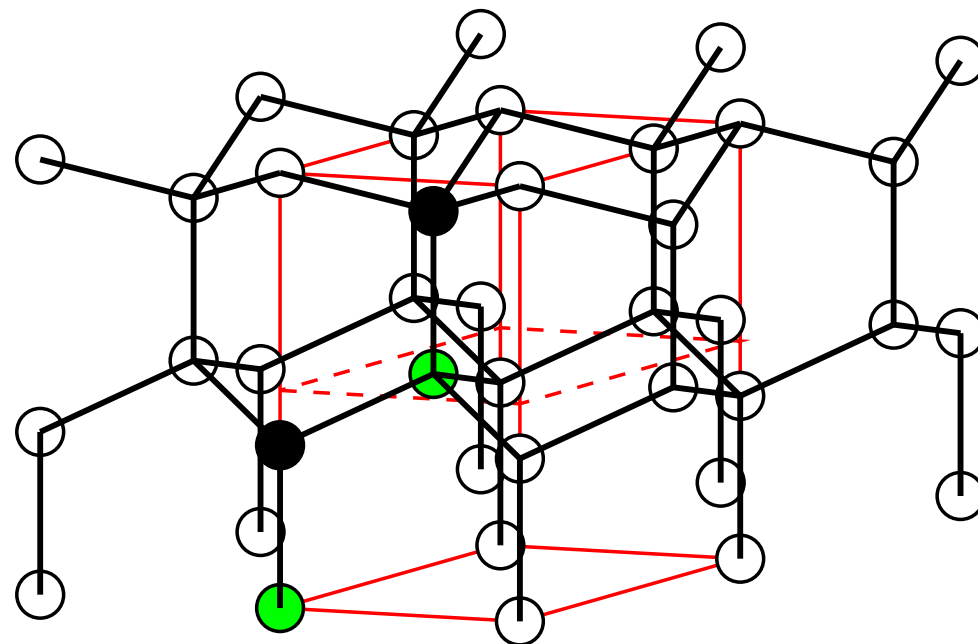
ATOMIC_POSITIONS crystal

Zn 0.0 0.0 0.0

Zn 0.33333333 0.66666666 0.5

O 0.0 0.0 0.345

O 0.66666666 0.33333333 0.845



ZnS: hexagonal \longrightarrow ibrav = 4

$a = 3.811 \text{ \AA}$, $c = 6.234 \text{ \AA} \longrightarrow c/a = 1.63579113$

$u = 0.375$

&SYSTEM

ntyp=2, nat=4, ibrav=4, a = 3.811, c = 6.234,

/

...

ATOMIC_SPECIES

Zn 1. Zn.UPF

S 1. S.UPF

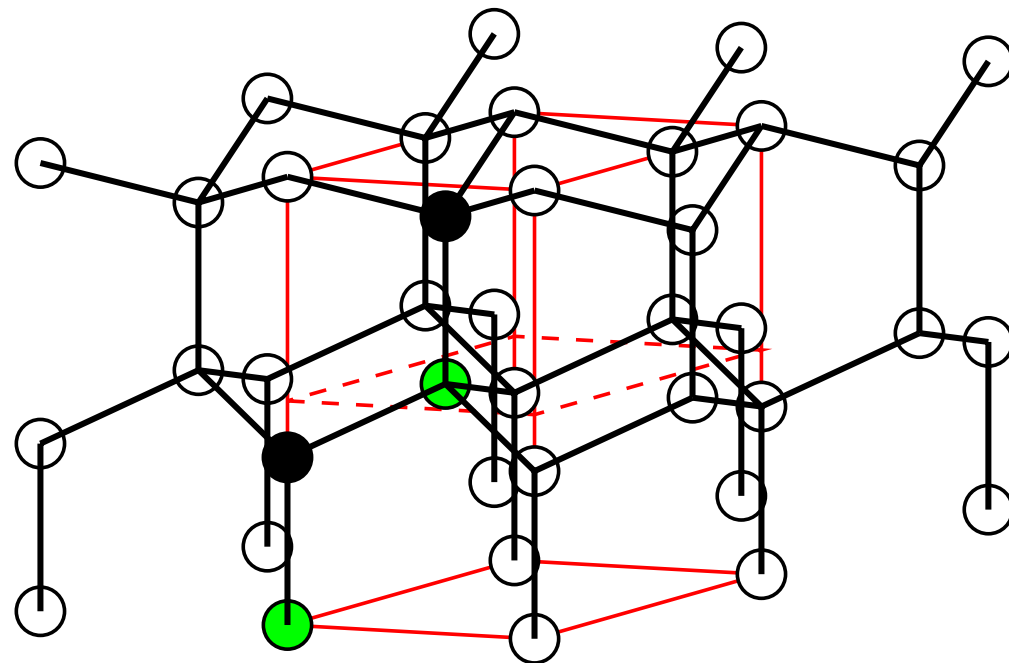
ATOMIC_POSITIONS crystal

Zn 0.0 0.0 0.0

Zn 0.33333333 0.66666666 0.5

S 0.0 0.0 0.375

S 0.66666666 0.33333333 0.875



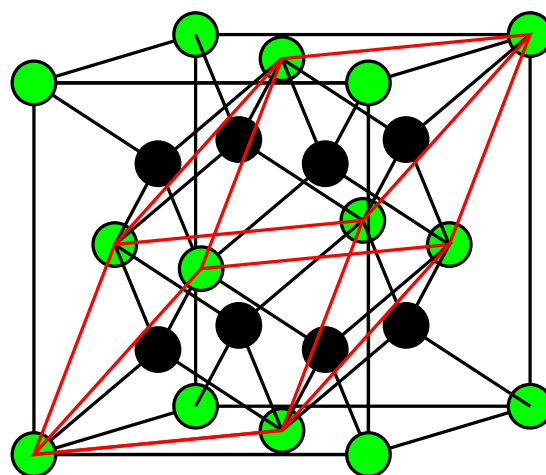
fluorite

IV,a1: Crystals RX_2 in which R is especially big are likely to have the *fluorite*, CaF_2 , arrangement. In this grouping each R atom is at the center of eight X atoms situated at the corners of a surrounding cube; and each X atom has about it a tetrahedron of R atoms. The symmetry is cubic with the atoms of its four molecules per unit in the following positions of O_h^5 ($Fm\bar{3}m$):

R: (4a) 000; F.C.

X: (8c) $\pm(1/4 \ 1/4 \ 1/4)$; FC

Crystal	a_0 Å
CaF_2	5.46295 (28 °C)
CeO_2	5.4110 (26 °C)



CaF₂: simple cubic \longrightarrow ibrav = 1

5.46295 Å \longrightarrow celldm(1)=10.32348344 bohr

&SYSTEM

ntyp=2, nat=12, ibrav=1, celldm(1) = 10.32348344

/

...

ATOMIC_SPECIES

Ca 1. Ca.UPF

F 1. F.UPF

ATOMIC_POSITIONS

Ca 0.0 0.0 0.0

Ca 0.0 0.5 0.5

Ca 0.5 0.0 0.5

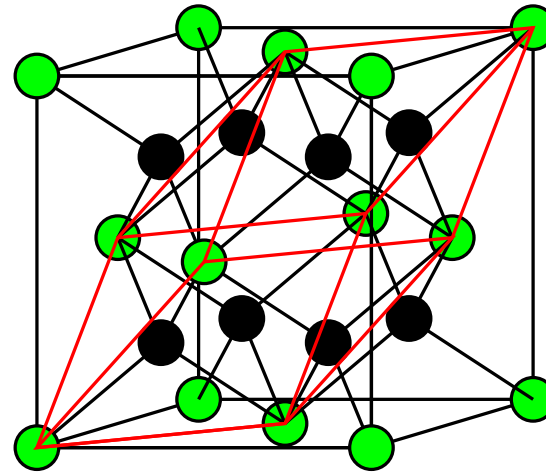
Ca 0.5 0.5 0.0

F 0.25 0.25 0.25

...

F -0.25 -0.25 -0.25

...



CaF₂: face centered cubic \longrightarrow ibrav = 2

5.46295 Å \longrightarrow celldm(1)=10.32348344 bohr

&SYSTEM

ntyp=2, nat=3, ibrav=1, celldm(1) = 10.32348344

/

...

ATOMIC_SPECIES

Ca 1. Ca.UPF

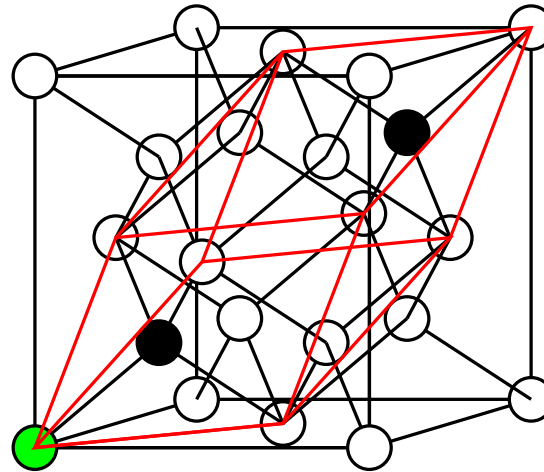
F 1. F.UPF

ATOMIC_POSITIONS

Ca 0.0 0.0 0.0

F 0.25 0.25 0.25

F -0.25 -0.25 -0.25



lanthanum sesquioxide

V,a1: A number of rare-earth oxides with large metal-to-oxygen separations form hexagonal crystals of which *lanthanum sesquioxide*, La_2O_3 , is typical. Assuming that the atoms have the dimensions of their ions, these are compounds with $r(\text{R})/r(\text{O})$ greater than 0.87. There is but one molecule in the unit which for La_2O_3 has the cell edges:

$$a_0 = 3.9373 \text{ \AA}, c_0 = 6.1299 \text{ \AA}$$

The space group is $D_{3d}^3 (C\bar{3}m)$ and the atoms are in the positions:

La: $(2d) \pm (1/3 \ 2/3 \ u)$ with $u = 0.245$ (from neutron diffraction)

O(1): $(1a) \ 000$ and O(2) $(2d)$ with $u = 0.645$

In this arrangement each lanthanum has four oxygen neighbors at a distance of ca 2.30 Å and three more at ca 2.70 Å. The oxygen atoms have their usual ionic separation with the closest O-O = ca 2.75 Å.

Crystal	a_0 , Å	c_0 , Å
Ce_2O_3	3.888	6.069

La₂O₃: hexagonal \longrightarrow ibrav = 4
a = 3.9373 Å, c = 6.1299 Å
 $u_{La} = 0.245$, $u_O = 0.645$

&SYSTEM

ntyp=2, nat=5, ibrav=4, a = 3.9373, c = 6.1299

/

...

ATOMIC_SPECIES

La 1. La.UPF

O 1. O.UPF

ATOMIC_POSITIONS crystal

La 0.33333333 0.66666666 0.245

La -0.33333333 -0.66666666 -0.245

O 0.0 0.0 0.0

O 0.33333333 0.66666666 0.645

O -0.33333333 -0.66666666 -0.645

corundum

V,a3: With smaller metallic atoms which make $r(R)/r(O)$ less than 0.60, oxygen ions can approach nearer to a perfect close-packing than is the case with preceding two structures, and such oxides are often found with an arrangement typified by that of *chromium sesquioxide*, Cr_2O_3 . Its symmetry is rhombohedral with a unit cell containing two molecules and having the dimensions:

$$a_0 = 5.350 \text{ \AA}, \alpha = 55^\circ 9'$$

The space group is $D_{3d}^6 (R\bar{3}c)$ and atoms are in the special positions:

Cr: (4c) $\pm (uuu)$; BC. with $u = 0.3475$

O: (6e) $\pm (u, 1/2-u, 1/4; 1/2-u, 1/4, u; 1/4, u, 1/2-u)$ with $u=0.556$

The dimensions of the corresponding hexamolecular cell referred to hexagonal axes are

$$a'_0 = 4.954 \text{ \AA}, c'_0 = 13.584 \text{ \AA}.$$

In this cell the atoms have the positions:

Cr: (12c) $\pm (00u', 0, 0, u'+1/2)$; rh with $u'=0.3475$

O : (18e) $\pm (v \ 0 \ 1/4; 0 \ v \ 1/4; \bar{v} \ \bar{v} \ 1/4)$; rh with $v=0.306$

[rh means repeat about $1/3$ $2/3$ $2/3$ and $2/3$ $1/3$ $1/3$]

Compound	$u=u'(R)$	$u(O)$	$v(O)$
Al_2O_3	0.3520	0.556	0.306
$\alpha\text{-Fe}_2O_3$	0.355	0.550	0.300
Ti_2O_3	0.3450	0.567	0.317
V_2O_3	0.3463	0.565	0.315

Crystal	a_0 Å	α	a'_0 Å	c'_0 Å
Al_2O_3 (corundum)	5.128	$55^\circ 20'$	4.76280	13.00320
$\alpha\text{-Fe}_2O_3$ (hematite)	5.4135	$55^\circ 17'$	5.035	13.72
Ti_2O_3	5.431	$56^\circ 36'$	5.148	13.636
VI_2O_3	5.647	$53^\circ 45'$	5.105	14.449

THE END