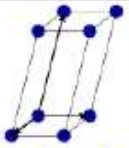
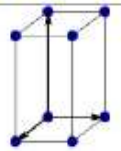
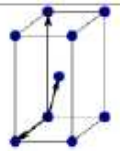
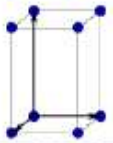
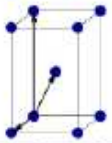
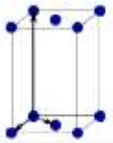
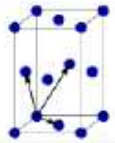
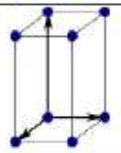
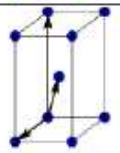
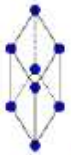
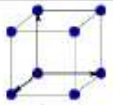
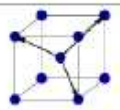
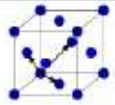
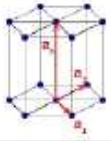
from Wyckoff to Quantum ESPRESSO

How to translate a crystallografic 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 ?

7 Crystal classes

14 Bravais lattice	Parameters	Simple (P)	Volume centered (I)	Base centered (C)	Face centered (F)
Triclinic	$a_1 \neq a_2 \neq a_3$ $\alpha_{12} \neq \alpha_{23} \neq \alpha_{31}$				
Monoclinic	$a_1 \neq a_2 \neq a_3$ $\alpha_{23} = \alpha_{31} = 90°$ $\alpha_{12} \neq 90°$				
Orthorhombic	$a_1 \neq a_2 \neq a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90°$				
Tetragonal	$a_1 = a_2 \neq a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90°$				
Trigonal	$a_1 = a_2 = a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} < 120°$				
Cubic	$a_1 = a_2 = a_3$ $\alpha_{12} = \alpha_{23} = \alpha_{31} = 90°$				
Hexagonal	$a_1 = a_2 \neq a_3$ $\alpha_{12} = 120°$ $\alpha_{23} = \alpha_{31} = 90°$				

The &SYSTEM namelist (STRUCTURE)

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


  0       read unit cell information from CELL_PARAMETRES 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,...,6
2)  a, b, c, cosab, cosac, cosbc,
```

```
celldm(1) = a / bohr_radius_angs = alat (internal unit of lenght)
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

ibrav	celldm -->	a = 1	b = 2	c = 3	cosab = 4	cosac = 5	cosbc = 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)$\neq$0, lattice vectors are given in these units

If celldm(1)=0, lattice vectors are given in BOHR, and the lenght 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, nbnd = 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 specify 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 specify 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

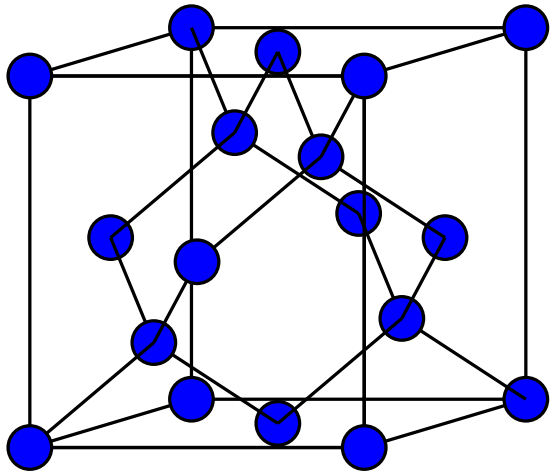
II,i1: The unit cubes of crystals with the *diamond structure* have eight atoms in the position of O_h^7 $(Fd3m)$:

```
(8a) 000;0 1/2 1/2; 1/2 0 1/2; 1/2 1/2 0;
        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 more briefly

```
(8a) 000; 1/4 1/4 1/4; F.C.
```

Element	Name	a_0, A
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

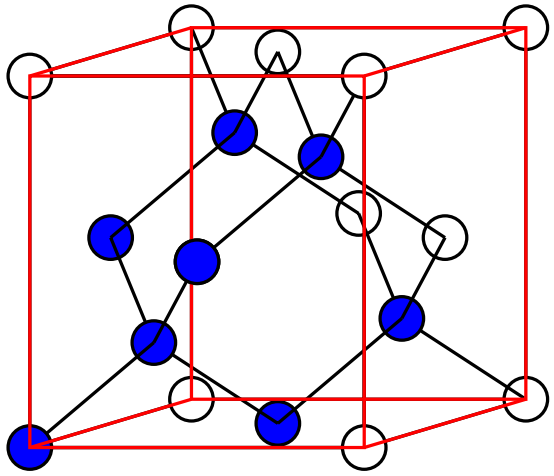
II,i1: The unit cubes of crystals with the *diamond structure* have eight atoms in the position of O_h^7 $(Fd3m)$:

```
(8a) 000;0 1/2 1/2; 1/2 0 1/2; 1/2 1/2 0;
          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 more briefly

```
(8a) 000; 1/4 1/4 1/4; F.C.
```

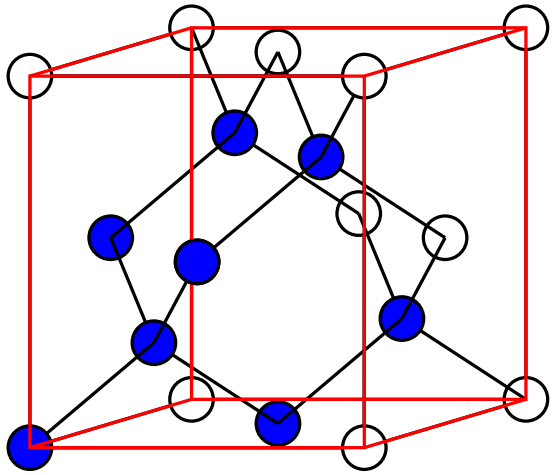
Element	Name	a_0, A
C	carbon	3.56679 (20 C)
Si	Silicon	5.43070 (25 C)
		5.445 (1300 C)
Ge	Germanium	5.65735 (20 C)
		5.65695 (18 C)
α-Sn	Tin (gray)	6.4912



C: simple cubic $\longrightarrow$ ibrav $= 1$

3.56679 A

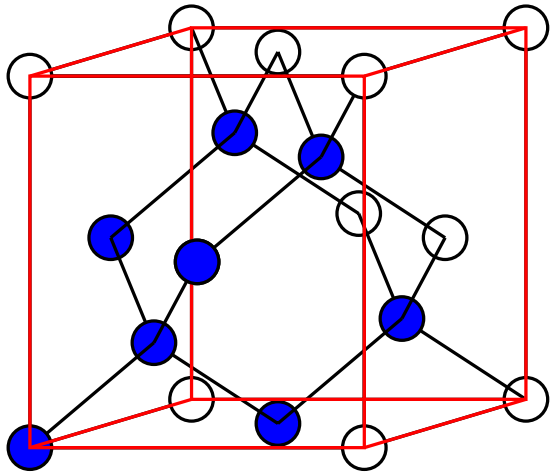
```
 &SYSTEM
    ntyp=1, nat=8, ibrav=1, a =  3.56679,
 /
...
ATOMIC_SPECIES
C 28.086 C.UPF
ATOMIC_POSITIONS
C 0.0 0.0 0.0
C 0.0 0.5 0.5
C 0.5 0.0 0.5
C 0.5 0.5 0.0
C 0.25 0.25 0.25
C 0.25 0.75 0.75
C 0.75 0.25 0.75
C 0.75 0.75 0.25
```



C: simple cubic $\longrightarrow$ ibrav = 1

3.56679 A $\longrightarrow$ 6.740259 bohrs

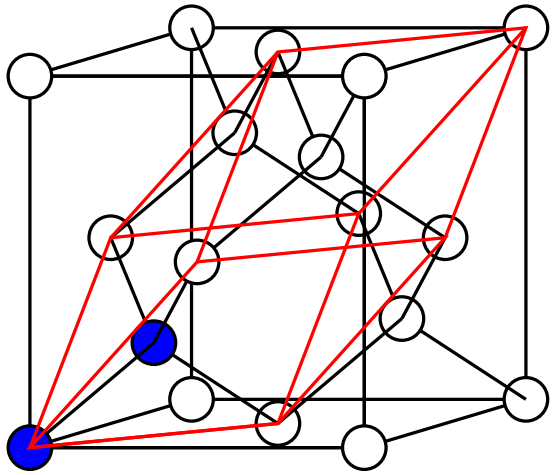
```
&SYSTEM
    ntyp=1, nat=8, ibrav=1, celldm(1)=6.740259,
/
...
ATOMIC_SPECIES
C 28.086 C.UPF
ATOMIC_POSITIONS
C 0.0 0.0 0.0
C 0.0 0.5 0.5
C 0.5 0.0 0.5
C 0.5 0.5 0.0
C 0.25 0.25 0.25
C 0.25 0.75 0.75
C 0.75 0.25 0.75
C 0.75 0.75 0.25
```



C: simple cubic $\longrightarrow$ ibrav $= 1$

3.56679 A $\longrightarrow$ 6.740259 bohrs

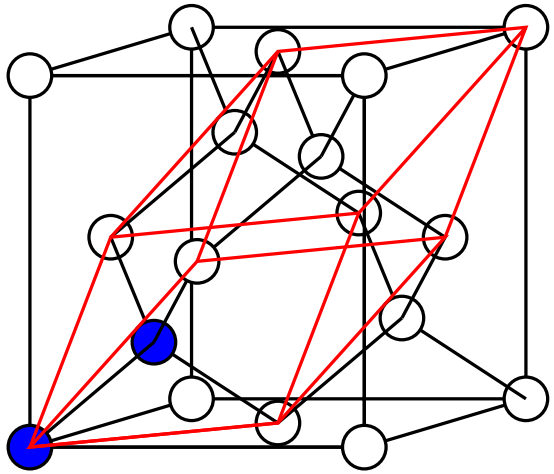
```
&SYSTEM
    ntyp=1, nat=8, ibrav=1, celldm(1)=6.740259,
/
...
ATOMIC_SPECIES
C 28.086 C.UPF
ATOMIC_POSITIONS
C 0.0 0.0 0.0
C 0.0 0.5 0.5
C 0.5 0.0 0.5
C 0.5 0.5 0.0
C 0.25 0.25 0.25
C 0.25 0.75 0.75
C 0.75 0.25 0.75
C 0.75 0.75 0.25
```



C: face centered cubic $\longrightarrow$ ibrav = 2

3.56679 A $\longrightarrow$ 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

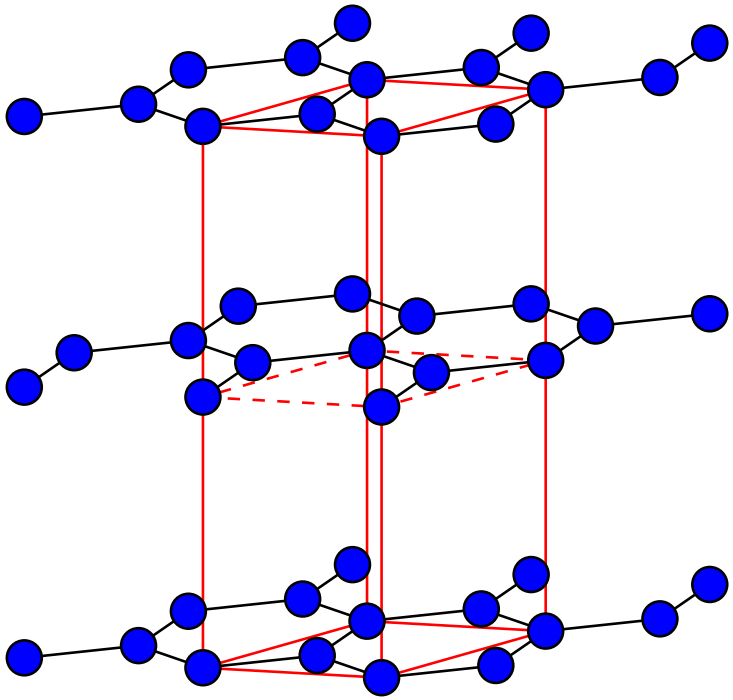
II,i2: The long-familiar form of *graphite* has an hexagonal unit with

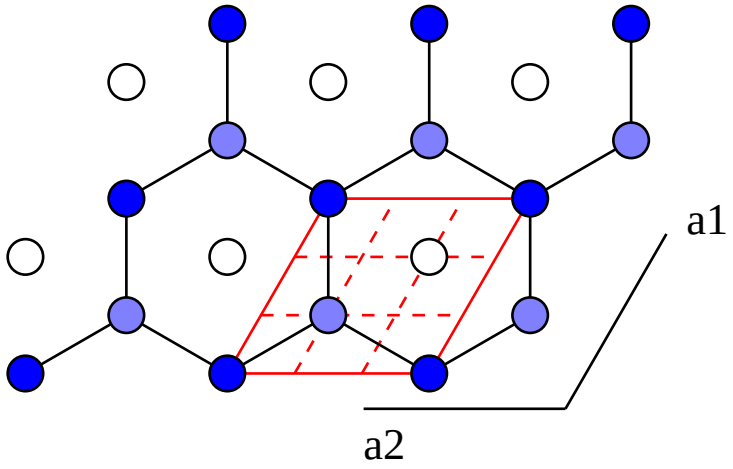
$a_0 = 2.456$ A, $c_0 = 6.696$ A

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

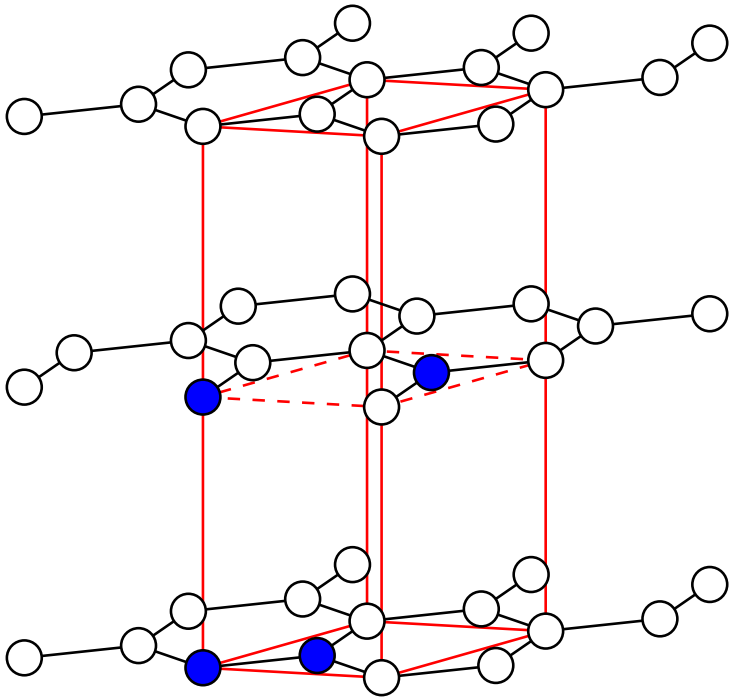
II,i2: The long-familiar form of *graphite* has an hexagonal unit with

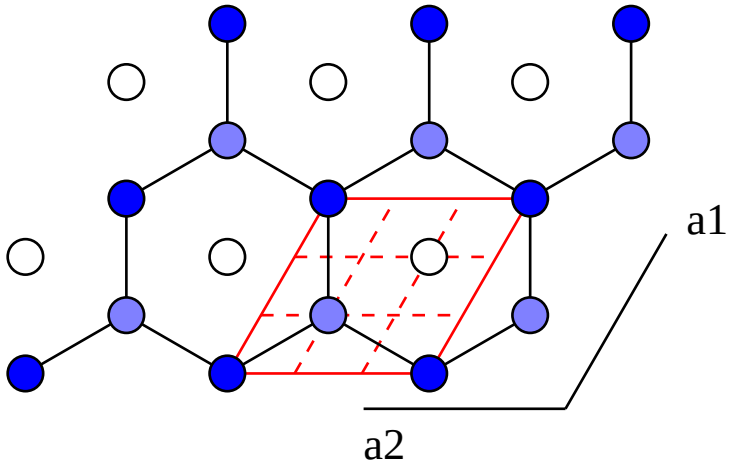
$a_0 = 2.456$ A, $c_0 = 6.696$ A

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



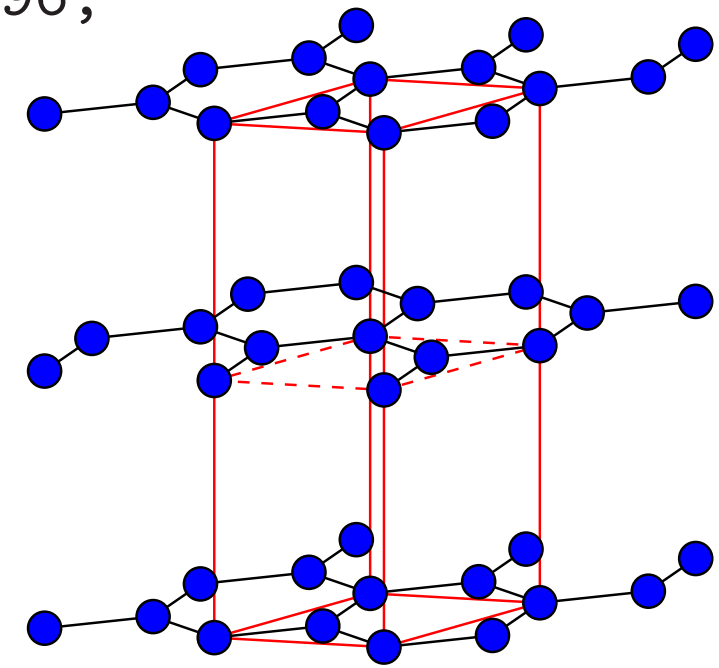


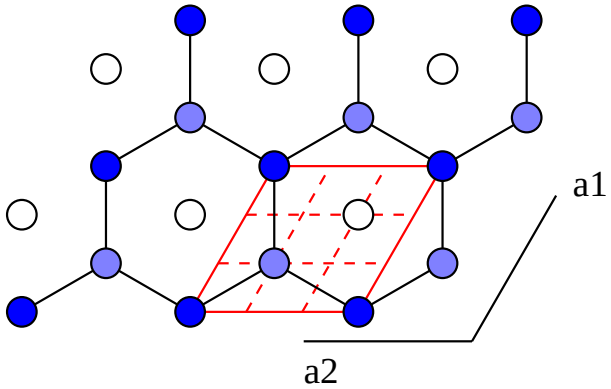
hexagonal $\longrightarrow$ ibrav = 4

a = 2.456 A, c = 6.696 A

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 0.333333333 0.666666666 0.0
C 0.0 0.0 0.5
C 0.666666666 0.333333333 0.5
```



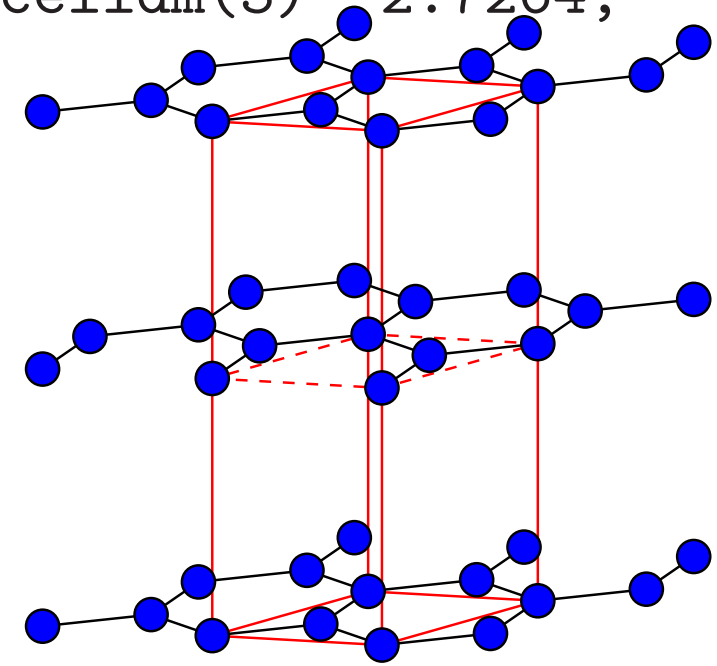


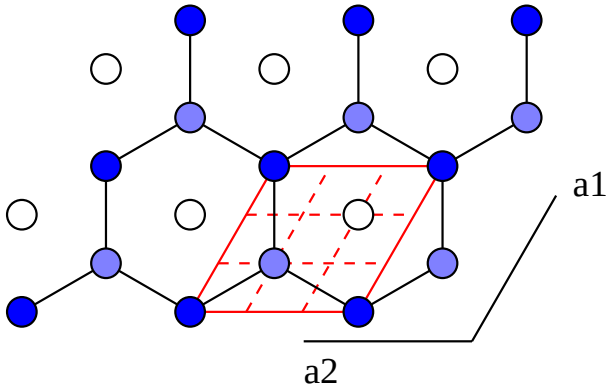
hexagonal $\longrightarrow$ ibrav = 4

a = 2.456 A, c = 6.696 A $\longrightarrow$ a = 4.64117 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 0.333333333 0.666666666 0.0
C 0.0 0.0 0.5
C 0.666666666 0.333333333 0.5
```



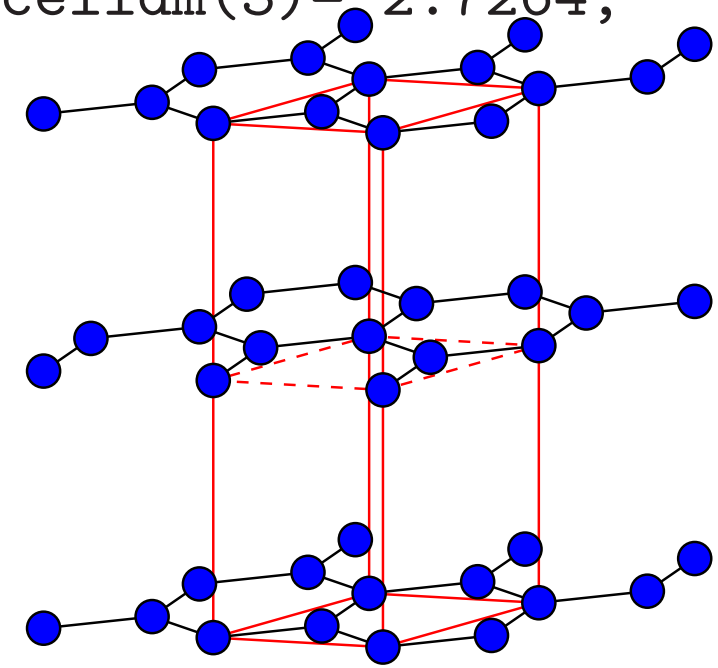


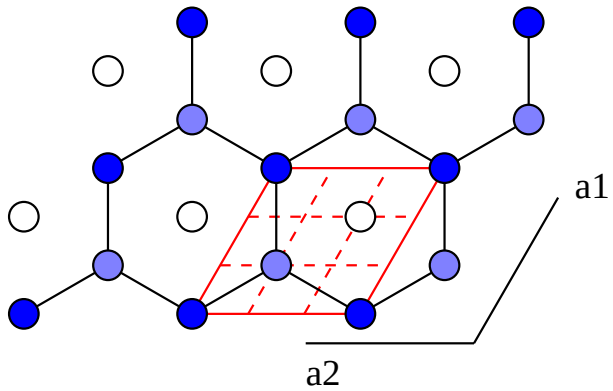
hexagonal $\longrightarrow$ ibrav = 4

a = 2.456 A, c = 6.696 A $\longrightarrow$ a = 4.64117 bohrs, c/a = 2.7264

u = v = 0 0.5 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
```



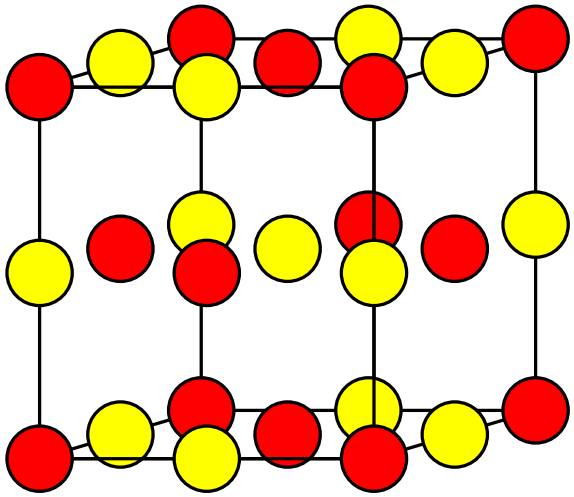


sodium cloride

III, a1: The largest group of RX-type crystals have the structure of *sodium cloride*, 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
....	

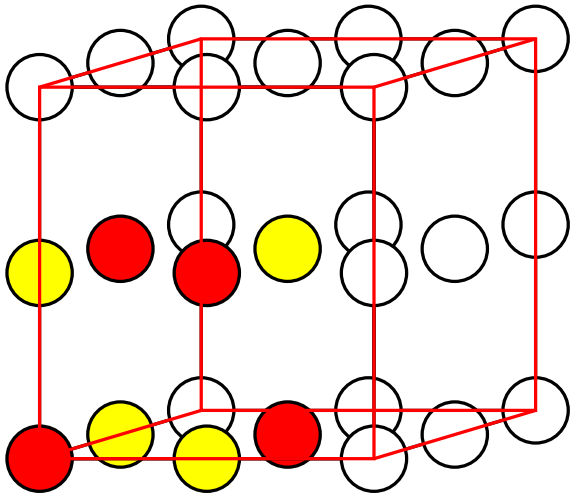


sodium cloride

III, a1: The largest group of RX-type crystals have the structure of *sodium cloride*, 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

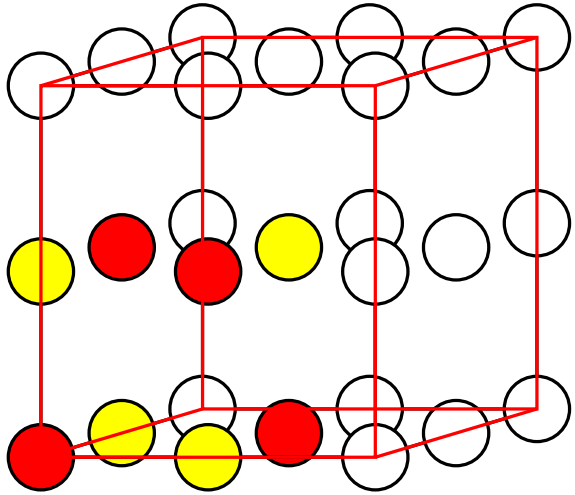
Crystal	a_0 A
....	
MgO	4.21112 (21 C)
....	
NaCl	5.62779 (18 C)
....	
NiO	4.1684
....	



MgO: face centered cubic $\longrightarrow$ ibrav = 2

4.21112 A $\longrightarrow$ 7.957867 bohrs

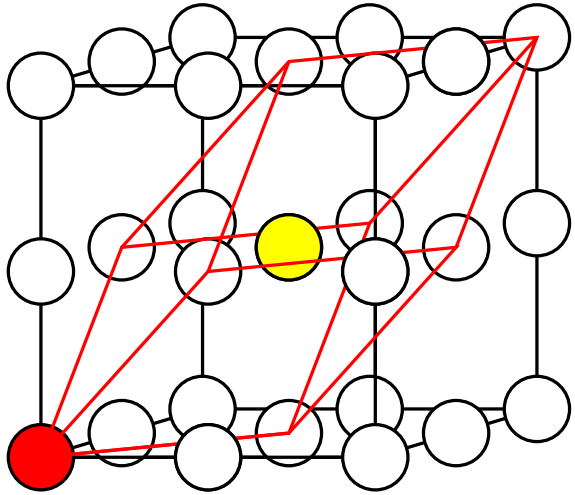
```
 &SYSTEM
    ntyp=2, nat=2, ibrav=2, celldm(1)=7.957867,
 /
...
ATOMIC_SPECIES
Mg 28.086 Mg.UPF
O  16.000 O.UPF
ATOMIC_POSITIONS
Mg 0.0 0.0 0.0
O  0.5 0.5 0.5
```



NiO: face centered cubic $\longrightarrow$ ibrav = 2

4.1684 A $\longrightarrow$ 7.87714 bohrs

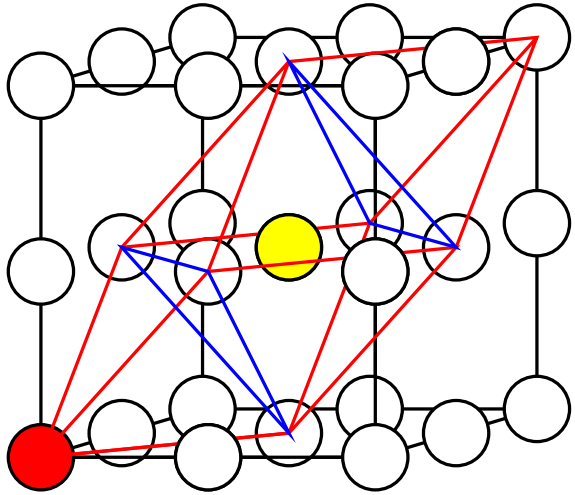
```
 &SYSTEM
    ntyp=2, nat=2, ibrav=2, celldm(1)= 7.87714,
 /
...
ATOMIC_SPECIES
Ni 28.086 Ni.UPF
O  16.000 O.UPF
ATOMIC_POSITIONS
Ni 0.0 0.0 0.0
O  0.5 0.5 0.5
```



NiO: face centered cubic $\longrightarrow$ ibrav = 2

4.1684 A $\longrightarrow$ 7.87714 bohrs

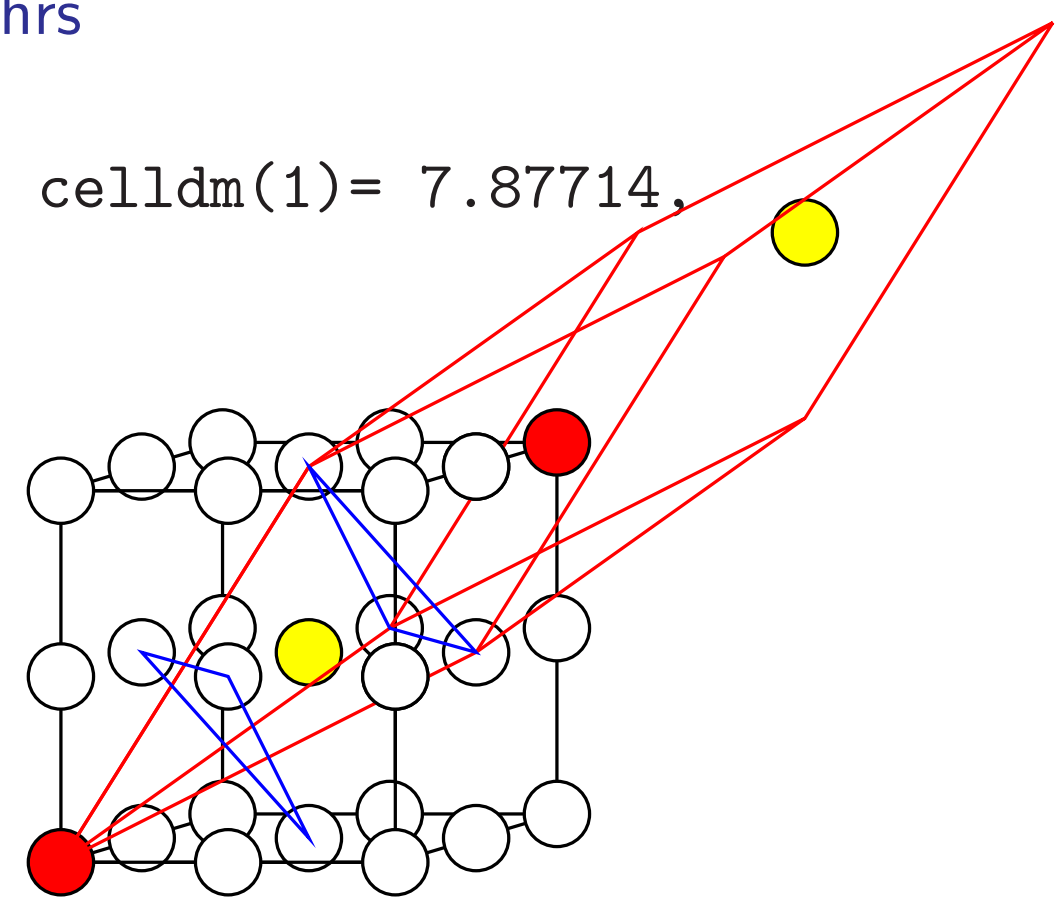
```
 &SYSTEM
    ntyp=2, nat=2, ibrav=2, celldm(1)= 7.87714,
 /
...
ATOMIC_SPECIES
Ni 28.086 Ni.UPF
O  16.000 O.UPF
ATOMIC_POSITIONS
Ni 0.0 0.0 0.0
O  0.5 0.5 0.5
```



NiO: face centered cubic $\longrightarrow$ ibrav = 2

4.1684 A $\longrightarrow$ 7.87714 bohrs

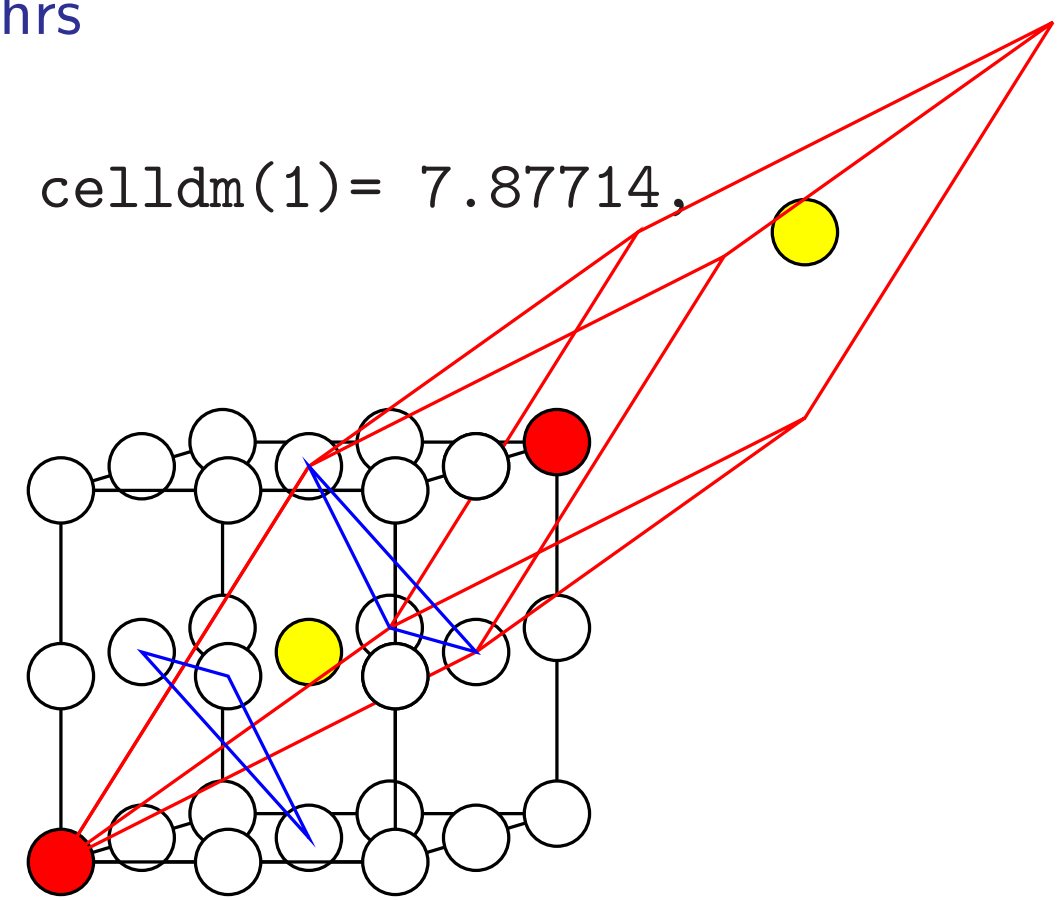
```
 &SYSTEM
    ntyp=2, nat=2, ibrav=2, celldm(1)= 7.87714,
 /
...
ATOMIC_SPECIES
Ni 28.086 Ni.UPF
O  16.000 O.UPF
ATOMIC_POSITIONS
Ni 0.0 0.0 0.0
O  0.5 0.5 0.5
```



NiO: user supplied lattice $\longrightarrow$ ibrav = 0

4.1684 A $\longrightarrow$ 7.87714 bohrs

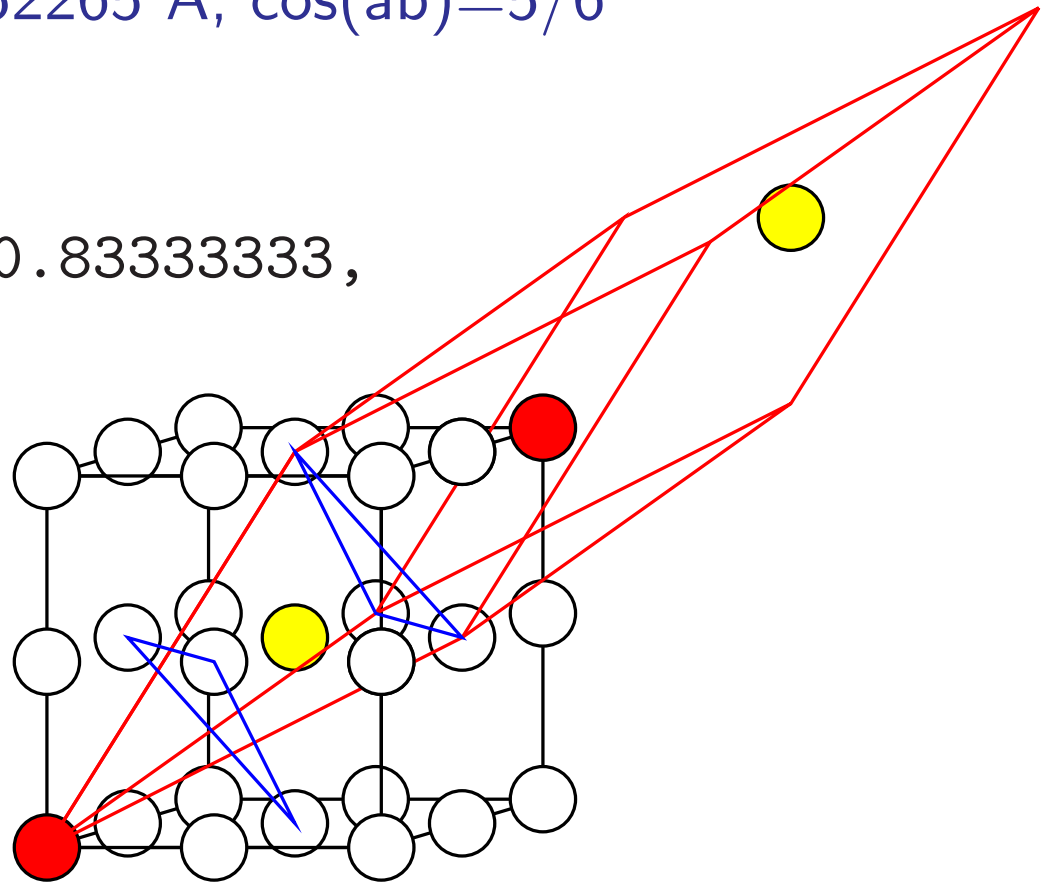
```
 &SYSTEM
    ntyp=3, nat=4, ibrav=0, celldm(1)= 7.87714,
 /
CELL_PARAMETERS cubic
1.00 0.50 0.50
0.50 1.00 0.50
0.50 0.50 1.00
ATOMIC_SPECIES
 Ni1  1.  Ni.UPF
 Ni2  1.  Ni.UPF
 O    1.  O.UPF
ATOMIC_POSITIONS crystal
 Ni1 0.0  0.0  0.0
 Ni2 0.5  0.5  0.5
 O  0.25 0.25 0.25
 O  0.75 0.75 0.75
```



NiO: rhombohedral lattice $\longrightarrow$ ibrav = 5

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

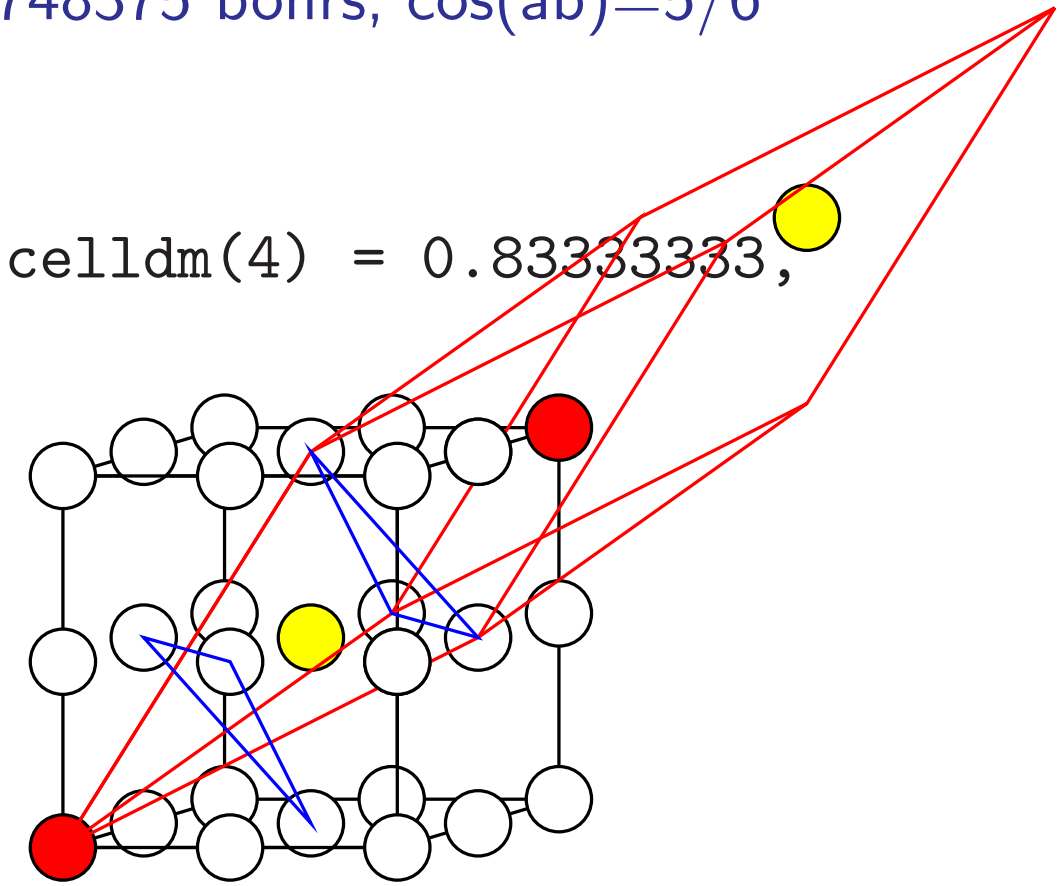
```
 &SYSTEM
    ntyp=3, nat=4, ibrav=5,
    a = 5.1052265, cosab = 0.83333333,
 /
ATOMIC_SPECIES
 Ni1  1.  Ni.UPF
 Ni2  1.  Ni.UPF
 O    1.  O.UPF
ATOMIC_POSITIONS crystal
 Ni1 0.0  0.0  0.0
 Ni2 0.5  0.5  0.5
 O  0.25 0.25 0.25
 O  0.75 0.75 0.75
```



NiO: rhombohedral lattice $\longrightarrow$ ibrav = 5

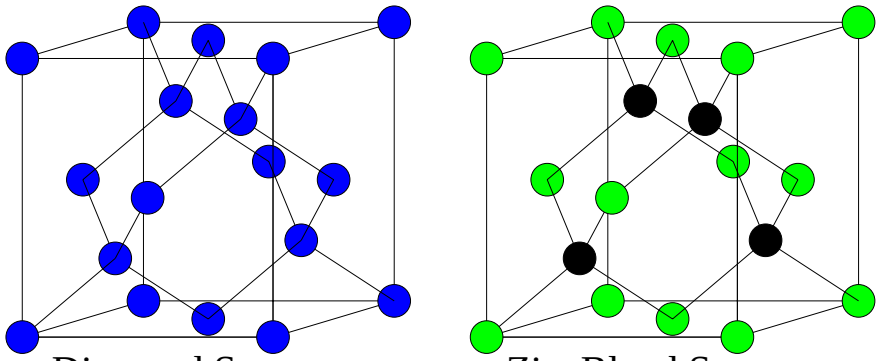
4.1684 A $\times\sqrt{3/2}$ = 9.64748375 bohrs, cos(ab)=5/6

```
 &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

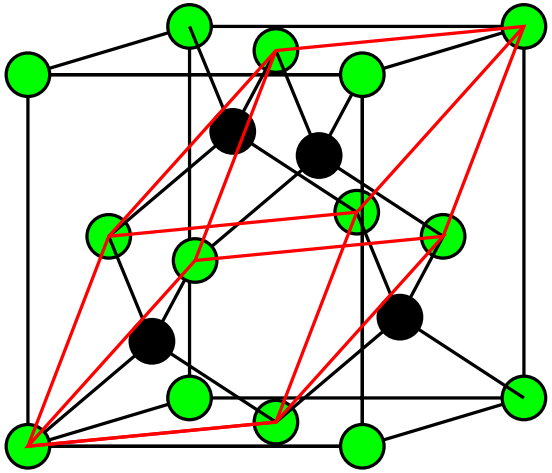
III, c1: The *zinc sulfide* arrangement, like that of NaCl contains four molecules in its unit cube and is developed on a face-centered lattice. Its atoms have the coordinates (of T_d^2 - $F\bar{4}3m$):
R: (4a) 000; 1/2 1/2 0; 1/2 0 1/2; 0 1/2 1/2, or 000; FC
X: (4c) 1/4 1/4 1/4; 1/4 3/4 3/4; 3/4 1/4 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 distamt 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

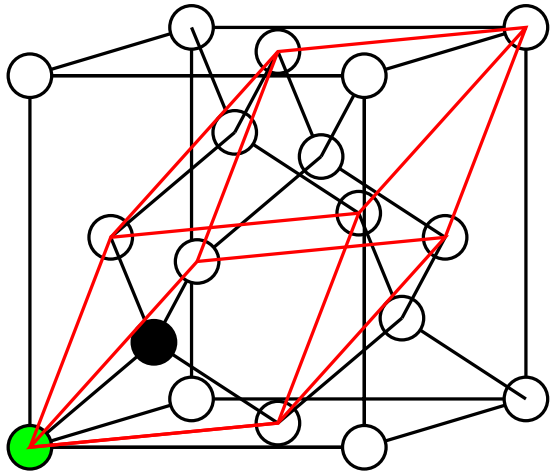
```
 &SYSTEM
    ntyp=2, nat=2, ibrav=2, celldm(1)=10.68,
 /
...
ATOMIC_SPECIES
Zn 1. Zn.UPF
S  1. S.UPF
ATOMIC_POSITIONS
Zn 0.0 0.0 0.0
S 0.25 0.25 0.25
```



ZnS: face centered cubic $\longrightarrow$ ibrav = 2

5.65 $\longrightarrow$ 10.68 bohrs

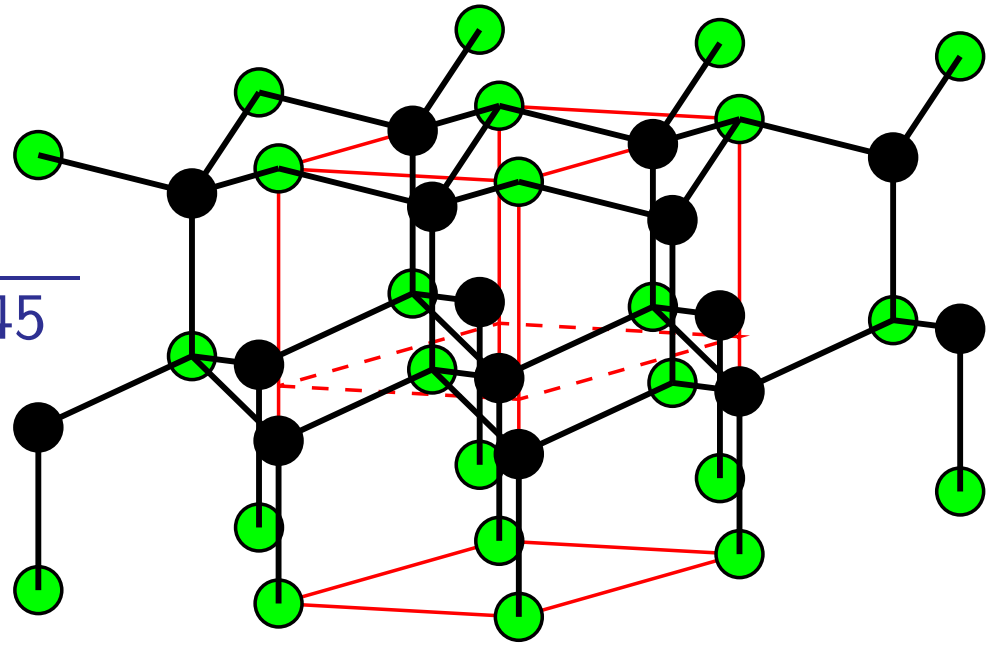
```
 &SYSTEM
    ntyp=2, nat=2, ibrav=2, celldm(1)=10.68,
 /
...
ATOMIC_SPECIES
Zn 1. Zn.UPF
S  1. S.UPF
ATOMIC_POSITIONS
Zn 0.0 0.0 0.0
S 0.25 0.25 0.25
```



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	

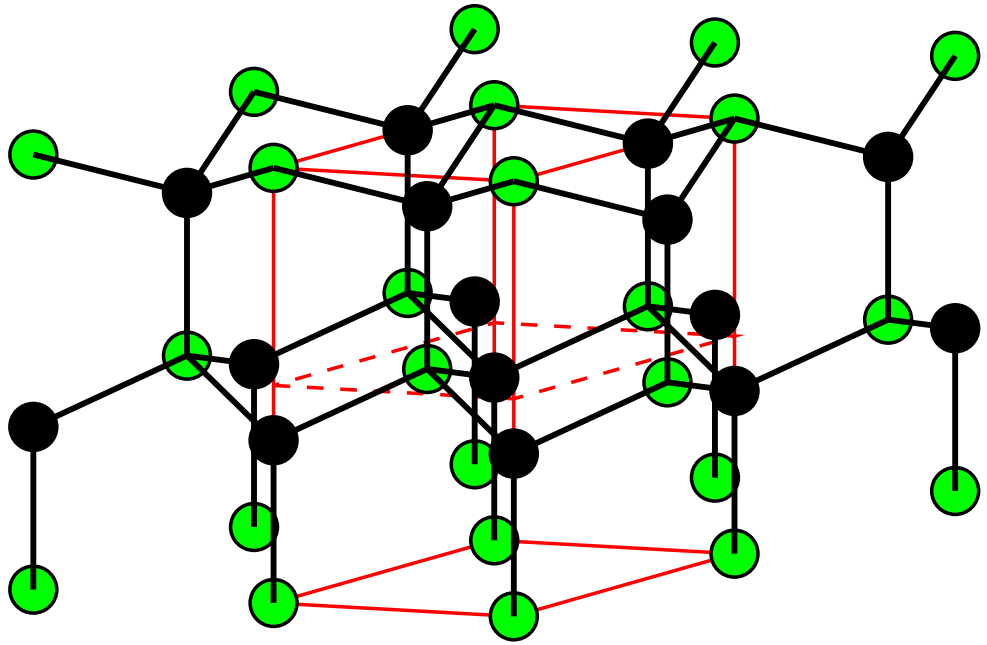


ZnO: hexagonal $\longrightarrow$ ibrav = 4

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  0.33333333 0.66666666 0.845
```

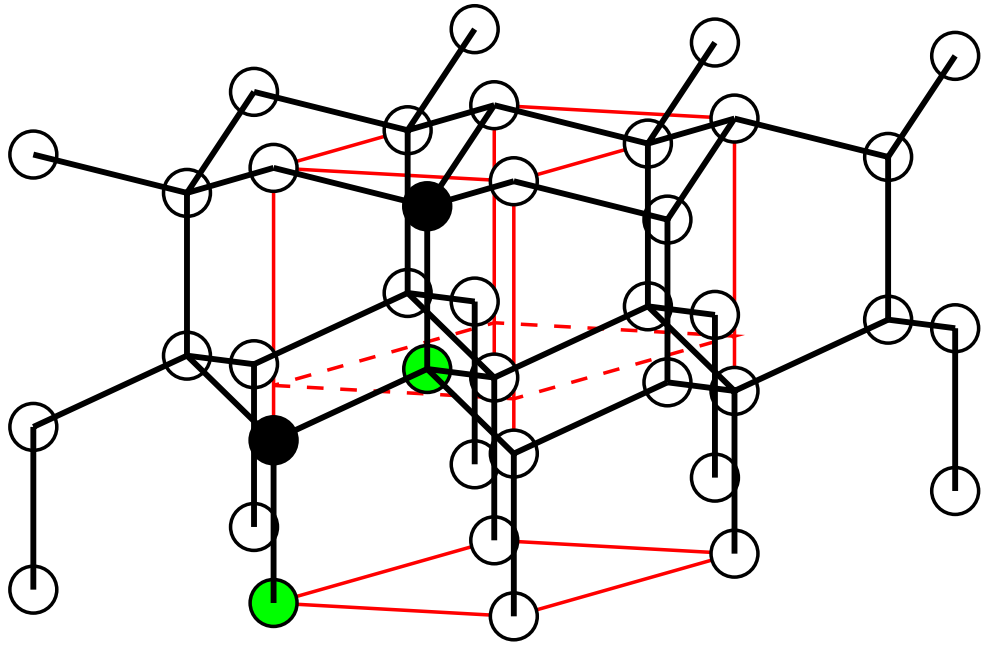


ZnO: hexagonal $\longrightarrow$ ibrav = 4

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  0.33333333 0.66666666 0.845
```

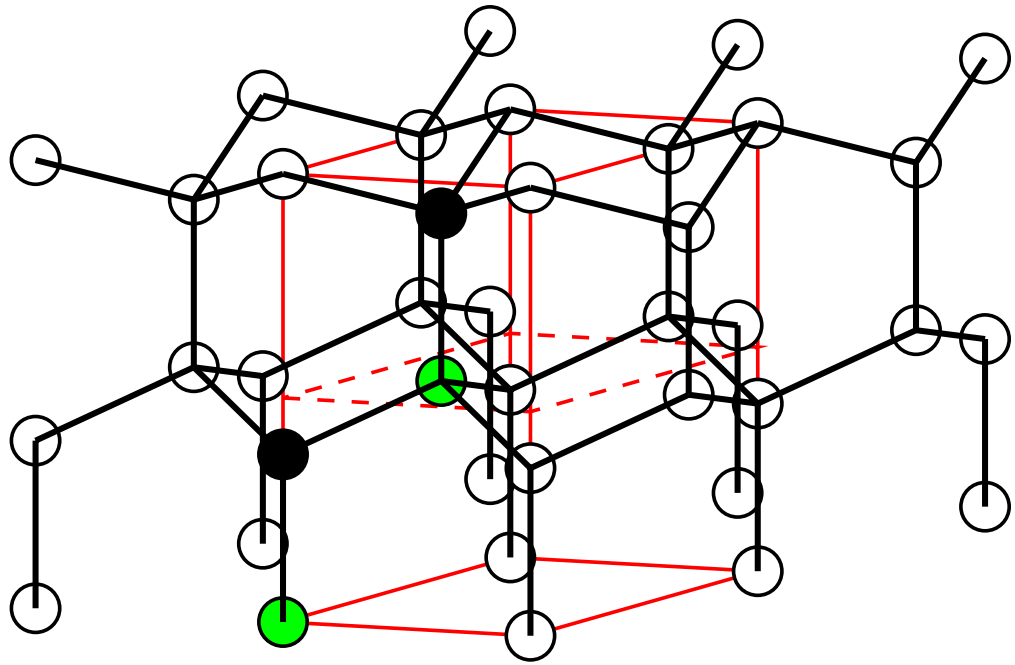


ZnS: hexagonal $\longrightarrow$ ibrav = 4

a = 3.811 A, c = 6.234 A $\longrightarrow$ 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  0.33333333 0.66666666 0.875
```



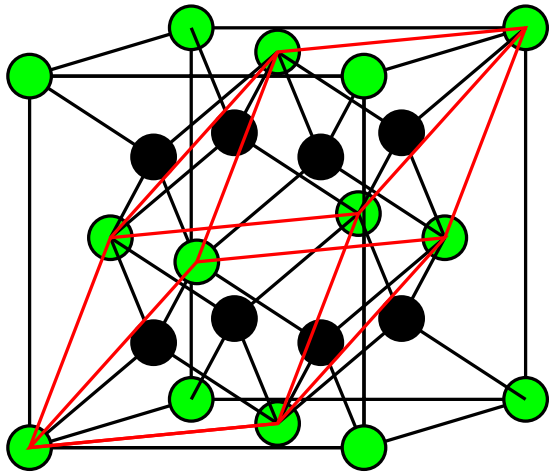
fluorite

IV,a1: Crystals RX_2 in which R is especially big are likely to have the *flourite*, 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 symmstry is cubic with the atoms of its four molecules per unit in the following positions of O_h^5 $(Fm3m)$:

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

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

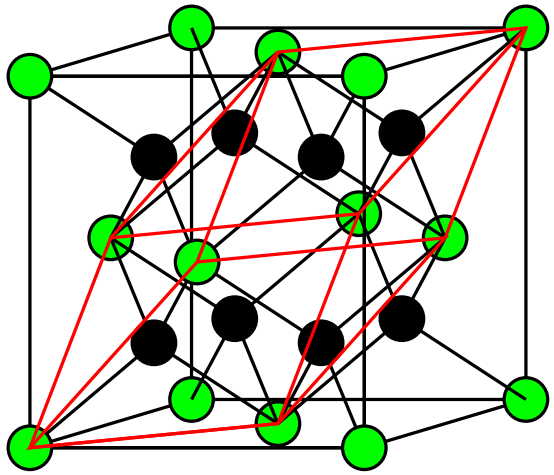
Crystal	a_0 A
CaF_2	5.46295 (28 C)
CeO_2	5.4110 (26 C)



CaF_2: simple cubic $\longrightarrow$ ibrav $= 1$

5.46295 A $\longrightarrow$ celldm(1)=10.32348344 bohr

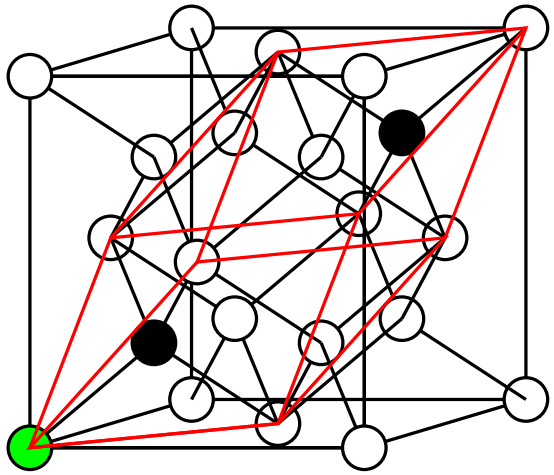
```
&SYSTEM
    ntyp=2, nat=12, ibrav=1, celldm(1) = 10.32348344
/
...
ATOMIC_SPECIES
Ca 1. Ca.UPF
F  1. F.UPF
ATOMIC_POSITIONS
Ca 0.0 0.0 0.0
Ca 0.0 0.5 0.5
Ca 0.5 0.0 0.5
Ca 0.5 0.5 0.0
F 0.25 0.25 0.25
...
F -0.25 -0.25 -0.25
...
```



CaF_2: face centered cubic $\longrightarrow$ ibrav $= 2$

5.46295 A $\longrightarrow$ 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 rate-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(R)/r(O) greater that 0.87. There is but one molecule in the unit which for La_2O_3 has the cell edges:

$$a_0 = 3.9373 \text{ A}, c_0 = 6.1299 \text{ A} .$$

The space group is D^3_{3d} $(C\bar{3}m)$ 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 A and three more at ca 2.70 A. The oxygen atoms have their usual ionic separation with the closest O-O = ca 2.75 A.

Crystal	a_0, A	c_0, A
Ce_2O_3	3.888	6.069

La_2O_3: hexagonal $\longrightarrow$ ibrav = 4

a = 3.9373 A, c = 6.1299 A

$u_{La} = 0.245$, $u_O = 0.645$

```
 &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 preceeding two structures, and such oxides are often found with an arrangement typified by that of *chromium sequioxide*, Cr_2O_3. Its symmetry is rhombohedral with a unit cell containing two molecules and having the dimensions:

$$a_0 = 5.350 \text{ A}, \alpha = 55^o9'$$

The space group is D^6_{3d} ($R\bar{3}c$) 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

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

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
α-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 A	α	a'$_0$ A	c'$_0$ A
Al_2O_3 (corundum)	5.128	55^o 20'	4.76280	13.00320
α-Fe_2O_3 (hematite)	5.4135	55^o 17'	5.035	13.72
Ti_2O_3	5.431	56^o 36'	5.148	13.636
Vl_2O_3	5.647	53^o 45'	5.105	14.449

THE END