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 CELLPARAMETRES 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)  \text{celldm}(i), i=1,2,...,6
2)  a, b, c, \cos(ab), \cos(ac), \cos(bc),

\text{celldm}(1) = a / \text{bohr}_\text{radius}_\text{angs} = \text{alat} \text{ (internal unit of length)}
\text{celldm}(2) = b / a
\text{celldm}(3) = c / a
\text{celldm}(4) = \cos(ab)
\text{celldm}(5) = \cos(ac)
\text{celldm}(6) = \cos(bc)

BEWARE:
alat = \text{celldm}(1) \text{ is the lattice parameter "a" in BOHR}
a,b,c \text{ 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

<table>
<thead>
<tr>
<th></th>
<th>Description</th>
<th>a</th>
<th>b</th>
<th>c</th>
<th>cosab</th>
<th>cosac</th>
<th>cosb</th>
<th>c</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>cubic P (sc)</td>
<td>*</td>
<td></td>
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<tr>
<td>2</td>
<td>cubic F (fcc)</td>
<td>*</td>
<td></td>
<td></td>
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<td></td>
</tr>
<tr>
<td>3</td>
<td>cubic I (bcc)</td>
<td>*</td>
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<td></td>
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<td></td>
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<tr>
<td>4</td>
<td>Hexagonal and Trigonal P</td>
<td>*</td>
<td>*</td>
<td></td>
<td></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>Trigonal R</td>
<td>*</td>
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<tr>
<td>6</td>
<td>Tetragonal P (st)</td>
<td>*</td>
<td>*</td>
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<tr>
<td>7</td>
<td>Tetragonal I (bct)</td>
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<td>*</td>
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<td></td>
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<td></td>
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<tr>
<td>8</td>
<td>Orthorhombic P</td>
<td>*</td>
<td>*</td>
<td>*</td>
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<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>Orthorhombic base-centered(bco)</td>
<td>*</td>
<td>*</td>
<td>*</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>Orthorhombic face-centered</td>
<td>*</td>
<td>*</td>
<td>*</td>
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<tr>
<td>11</td>
<td>Orthorhombic body-centered</td>
<td>*</td>
<td>*</td>
<td>*</td>
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<tr>
<td>12</td>
<td>Monoclinic P</td>
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<td>*</td>
<td>*</td>
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<td></td>
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<td></td>
<td></td>
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<tr>
<td>13</td>
<td>Monoclinic base-centered</td>
<td>*</td>
<td>*</td>
<td>*</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>Triclinic P</td>
<td>*</td>
<td>*</td>
<td>*</td>
<td>*</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
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 lenght of
the first lattice vector defines alat.
The &SYSTEM namelist (STRUCTURE) continued

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

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

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

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

\begin{verbatim}
ATOMIC_SPECIES
  X(1)    Mass_X(1)   PseudoPot_X(1)
  ...     
  X(ntyp) Mass_X(ntyp) PseudoPot_X(ntyp)
\end{verbatim}

example

\begin{verbatim}
ATOMIC_SPECIES
  0      16.00   O.LDA.US.RRKJ3.UPF
  C      12.00   C.pz-rrkjjus.UPF
\end{verbatim}
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
II,i1: The unit cubes of crystals with the *diamond structure* have eight atoms in the position of $O^7_h (Fd3m)$:

$$(8a) 000; 0 1/2 1/2; 1/2 0 1/2; 1/2 1/2 0;$$

$$(1/4 1/4 1/4; 1/4 3/4 3/4; 3/4 1/4 3/4; 3/4 3/4 1/4$$

or more briefly

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

<table>
<thead>
<tr>
<th>Element</th>
<th>Name</th>
<th>$a_0$, Å</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>carbon</td>
<td>3.56679 (20 C)</td>
</tr>
<tr>
<td>Si</td>
<td>Silicon</td>
<td>5.43070 (25 C)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>5.445 (1300 C)</td>
</tr>
<tr>
<td>Ge</td>
<td>Germanium</td>
<td>5.65735 (20 C)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>5.65695 (18 C)</td>
</tr>
<tr>
<td>$\alpha$-Sn</td>
<td>Tin (gray)</td>
<td>6.4912</td>
</tr>
</tbody>
</table>
The unit cubes of crystals with the *diamond structure* have eight atoms in the position of $O^7_h \ (Fd3m)$:

$\begin{align*}
(8a) & \ 000; 0 1/2 1/2; 1/2 0 1/2; 1/2 1/2 0; \\
& \ 1/4 1/4 1/4; 1/4 3/4 3/4; 3/4 1/4 3/4; 3/4 3/4 1/4
\end{align*}$

or more briefly

$\begin{align*}
(8a) & \ 000; 1/4 1/4 1/4; \text{ F.C.}
\end{align*}$

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<td>Tin (gray)</td>
<td>6.4912</td>
</tr>
</tbody>
</table>
C: simple cubic $\rightarrow$ ibrav = 1
3.56679 Å

&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 → ibrav = 1
3.56679 A → 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 → ibrav = 1
3.56679 A → 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  \( \rightarrow \) ibrav = 2
3.56679 Å  \( \rightarrow \) 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
Il,i2: The long-familiar form of graphite has an hexagonal unit with
\( a_0 = 2.456 \text{ A}, \ c_0 = 6.696 \text{ A} \)

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

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

(2a) 00\( u \); 0,0,\( u + 1/2 \) \quad \text{and} \quad (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 $\rightarrow$ 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 0.333333333 0.666666666 0.0
C 0.0 0.0 0.5
C 0.666666666 0.333333333 0.5
hexagonal $\rightarrow$ ibrav = 4

$a = 2.456 \text{ Å}, \ c = 6.696 \text{ Å}$ $\rightarrow$ $a = 4.64117 \text{ bohrs}, \ c/a = 2.7264$

$u = v = 0$

&SYSTEM

ibrav=4, celldm(1)=4.64117, celldm(3)=2.7264,
n typ=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 $\rightarrow$ ibrav = 4
a = 2.456 Å, c = 6.696 Å $\rightarrow$ 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
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

<table>
<thead>
<tr>
<th>Crystal</th>
<th>(a_0) (\text{A})</th>
</tr>
</thead>
<tbody>
<tr>
<td>MgO</td>
<td>4.21112 (21 C)</td>
</tr>
<tr>
<td>NaCl</td>
<td>5.62779 (18 C)</td>
</tr>
<tr>
<td>NiO</td>
<td>4.1684</td>
</tr>
<tr>
<td>....</td>
<td></td>
</tr>
</tbody>
</table>
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

<table>
<thead>
<tr>
<th>Crystal</th>
<th>$a_0$ Å</th>
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<tbody>
<tr>
<td>MgO</td>
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<td>5.62779 (18 C)</td>
</tr>
<tr>
<td>NiO</td>
<td>4.1684</td>
</tr>
</tbody>
</table>

[Diagram of sodium chlorine crystal structure]
MgO:  face centered cubic \(\rightarrow\) ibrav = 2
4.21112 A \(\rightarrow\) 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 $\rightarrow$ ibrav = 2
4.1684 A $\rightarrow$ 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 $\rightarrow$ ibrav = 2
4.1684 A $\rightarrow$ 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 $\rightarrow$ ibrav = 2
4.1684 Å $\rightarrow$ 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 \( \rightarrow \) ibrav = 0
4.1684 A \( \rightarrow \) 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
0 0.25 0.25 0.25
0 0.75 0.75 0.75
NiO: rhombohedral lattice $\rightarrow$ ibrav = 5

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

&SYSTEM

ntyp=3, nat=4, ibrav=5,
a = 5.1052265, $\cos(ab) = 0.83333333$,
/

ATOMIC_SPECIES
Ni1 1. Ni.UPF
Ni2 1. Ni.UPF
0 1. O.UPF

ATOMIC_POSITIONS crystal
Ni1 0.0 0.0 0.0 0.0
Ni2 0.5 0.5 0.5
0 0.25 0.25 0.25
0 0.75 0.75 0.75
NiO: rhombohedral lattice $\rightarrow$ ibrav = 5

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

&SYSTEM

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

\[
\text{celldm}(1) = 9.64748375, \quad \text{celldm}(4) = 0.83333333,
\]

/

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
0 0.25 0.25 0.25
0 0.75 0.75 0.75
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 $T^2_d\ -\ F\bar{4}3m$):

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 → ibrav = 2
5.65 → 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 $\rightarrow$ ibrav = 2

5.65 $\rightarrow$ 10.68 bohrs

&SYSTEM

ttyp=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 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.

<table>
<thead>
<tr>
<th>Crystal</th>
<th>$a_0$</th>
<th>$c_0$</th>
<th>remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>ZnO</td>
<td>3.24950</td>
<td>5.2069</td>
<td>$u = 0.345$</td>
</tr>
<tr>
<td>ZnS</td>
<td>3.811</td>
<td>6.234</td>
<td></td>
</tr>
</tbody>
</table>
ZnO: hexagonal $\rightarrow$ ibrav = 4
\[ a = 3.24950 \text{ Å}, \ c = 5.2069 \text{ Å} \rightarrow c/a=1.60236959 \]
\[ u = 0.345 \]

&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
0 0.0 0.0 0.345
0 0.66666666 0.33333333 0.845
ZnO: hexagonal $\rightarrow$ ibrav = 4
a = 3.24950 Å, c = 5.2069 Å $\rightarrow$ 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. 0.UPF
ATOMIC_POSITIONS crystal
Zn 0.0 0.0 0.0
Zn 0.33333333 0.66666666 0.5
0 0.0 0.0 0.345
0 0.66666666 0.33333333 0.845
ZnS: hexagonal $\rightarrow$ ibrav = 4

$a = 3.811$ Å, $c = 6.234$ Å $\rightarrow$ $c/a=1.63579113$

$u = 0.375$

&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
IV,a1: Crystals RX₂ in which R is especially big are likely to have the *fluorite*, CaF₂, 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 $O^5_h$ ($Fm3m$):

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

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

<table>
<thead>
<tr>
<th>Crystal</th>
<th>$a_0$ Å</th>
</tr>
</thead>
<tbody>
<tr>
<td>CaF₂</td>
<td>5.46295 (28 C)</td>
</tr>
<tr>
<td>CeO₂</td>
<td>5.4110 (26 C)</td>
</tr>
</tbody>
</table>
CaF$_2$: simple cubic $\rightarrow$ ibrav = 1
5.46295 Å $\rightarrow$ 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 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 $\rightarrow$ ibrav = 2
5.46295 Å $\rightarrow$ 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
V,a1: A number of rare-earth oxides with large metal-to-oxygen separations form hexagonal crystals of which lanthanum sesquioxide, La$_2$O$_3$, is typical. Assuming that the atoms have the dimensions of their ions, these are compounds with $r(R)/r(O)$ greater than 0.87. There is but one molecule in the unit which for La$_2$O$_3$ has the cell edges:

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

The space group is $D_{3d}^3 (C\bar{5}m)$ and the atoms are in the positions:

La: (2d) ± (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.

<table>
<thead>
<tr>
<th>Crystal</th>
<th>$a_0$, A</th>
<th>$c_0$, A</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ce$_2$O$_3$</td>
<td>3.888</td>
<td>6.069</td>
</tr>
</tbody>
</table>
La$_2$O$_3$: hexagonal $\rightarrow$ 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 sequioxide, $\text{Cr}_2\text{O}_3$. Its symmetry is rhombohedral with a unit cell containing two molecules and having the dimensions:

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

The space group is $D_{3d}^6 (R\overline{3}c)$ 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

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

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 ]

<table>
<thead>
<tr>
<th>Compound</th>
<th>$u=\mu'(R)$</th>
<th>$u(O)$</th>
<th>$v(O)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al$_2$O$_3$</td>
<td>0.3520</td>
<td>0.556</td>
<td>0.306</td>
</tr>
<tr>
<td>$\alpha$-Fe$_2$O$_3$</td>
<td>0.355</td>
<td>0.550</td>
<td>0.300</td>
</tr>
<tr>
<td>Ti$_2$O$_3$</td>
<td>0.3450</td>
<td>0.567</td>
<td>0.317</td>
</tr>
<tr>
<td>V$_2$O$_3$</td>
<td>0.3463</td>
<td>0.565</td>
<td>0.315</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Crystal</th>
<th>$a_0$ A</th>
<th>$\alpha$</th>
<th>$a'_0$ A</th>
<th>$c'_0$ A</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al$_2$O$_3$ (corundum)</td>
<td>5.128</td>
<td>55° 20'</td>
<td>4.76280</td>
<td>13.00320</td>
</tr>
<tr>
<td>$\alpha$-Fe$_2$O$_3$ (hematite)</td>
<td>5.4135</td>
<td>55° 17'</td>
<td>5.035</td>
<td>13.72</td>
</tr>
<tr>
<td>Ti$_2$O$_3$</td>
<td>5.431</td>
<td>56° 36'</td>
<td>5.148</td>
<td>13.636</td>
</tr>
<tr>
<td>Vl$_2$O$_3$</td>
<td>5.647</td>
<td>53° 45'</td>
<td>5.105</td>
<td>14.449</td>
</tr>
</tbody>
</table>
THE END