# MINERALS AND ROCKS

Exercises in Crystal and Mineral Chemistry, Crystallography, X-Ray Powder Diffraction, Mineral and Rock Identification, and Ore Mineralogy

Third Edition

*Solutions Manual*

Exercise 3

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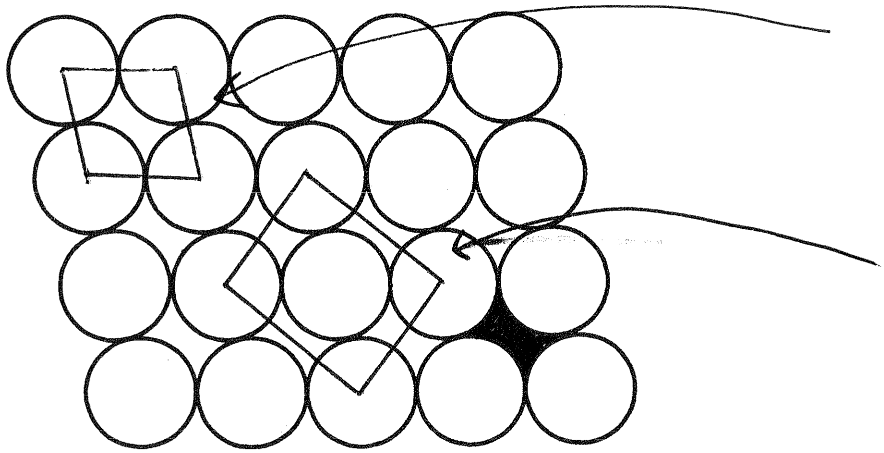
University of New Mexico

# EXERCISE 3

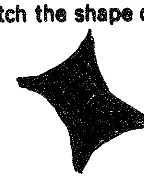
Student Name

**FIGURE 3.3** Assignment on two-dimensional packing of equally-sized spheres.

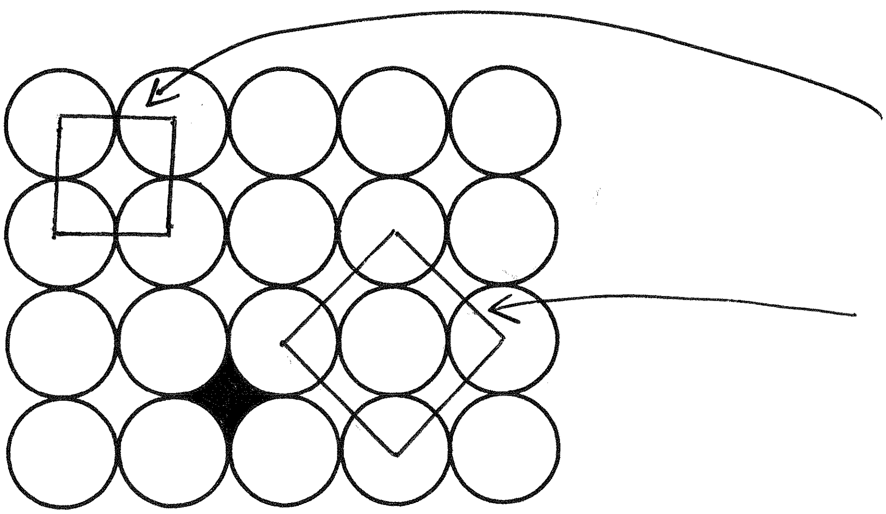
*(a)*



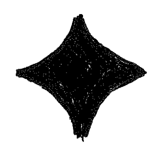
1. Geometry of array oblique
2. C.N. 4
3. In the array outline the shape of coordinating spheres
4. Sketch the shape of the interstice



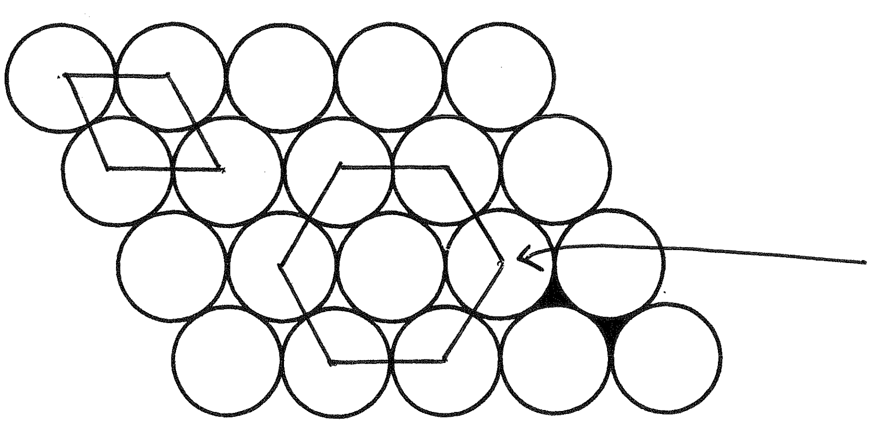
*(b)*



1. Geometry of array square
2. C.N. 4
3. In the array outline the shape of coordinating spheres
4. Sketch the shape of the interstice



*(c)*



1. Geometry of array hexagonal
2. C.N. 6
3. In the array outline the shape of coordinating spheres
4. Sketch the shape of the interstice

 or 

# EXERCISE 3

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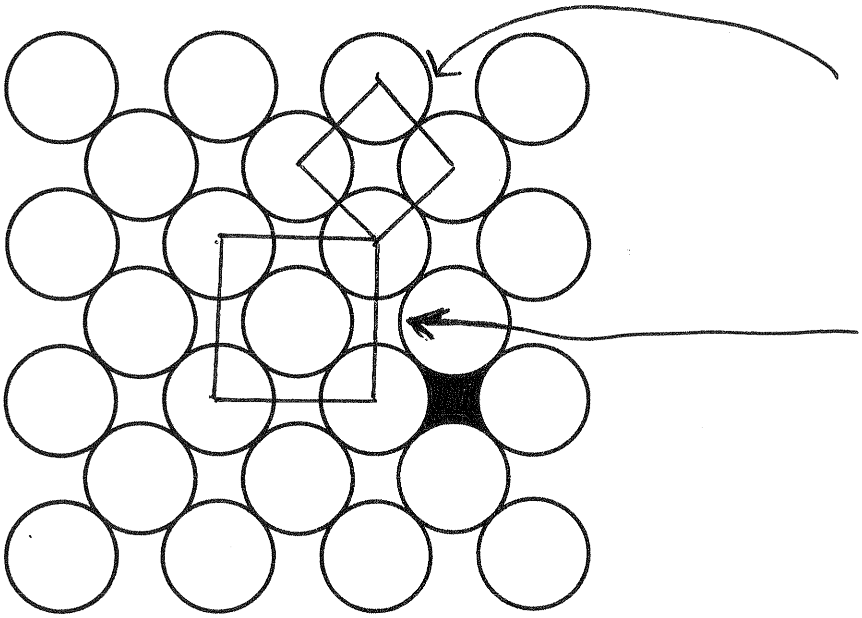
**FIGURE 3.3** *(continued)*

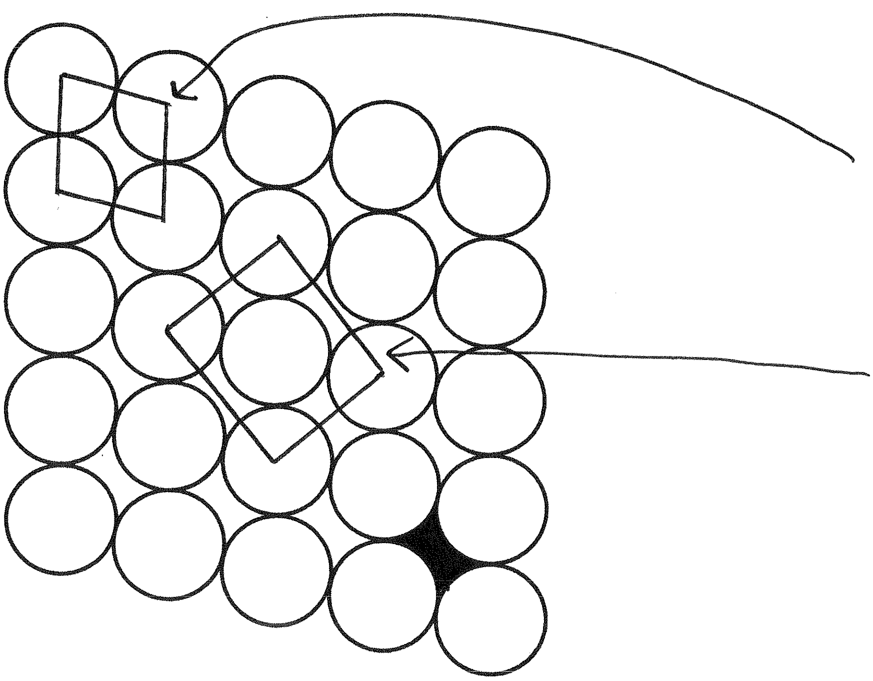
*(d)*



1. Geometry of array Square
2. C.N. 4
3. In the array outline the shape of coordinating spheres
4. Sketch the shape of the interstice

5. How does this array relate to that in fig. 3.3*b*?
45° rotation

*(e)*



1. Geometry of array oblique
2. C.N. 4
3. In the array outline the shape of coordinating spheres
4. Sketch the shape of the interstice

5. How does this array relate to that in fig. 3.3*a*?
~20° rotation

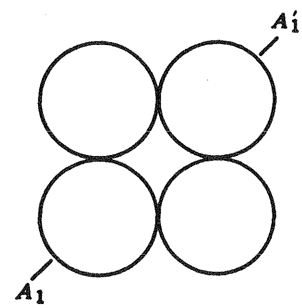
# EXERCISE 3

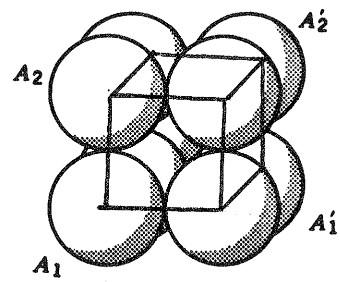
Student Name

**FIGURE 3.4** Assignment on three-dimensional packing of equally-sized spheres.

**Plan view** | **Three-dimentional stacking**

*(a)*



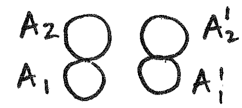




1. **Outline unit cell in model and give name of its shape**

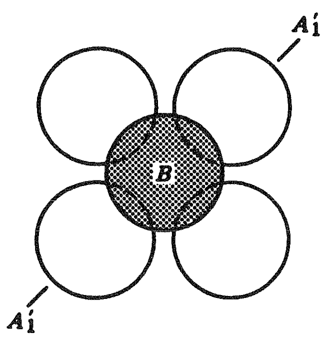
   cube

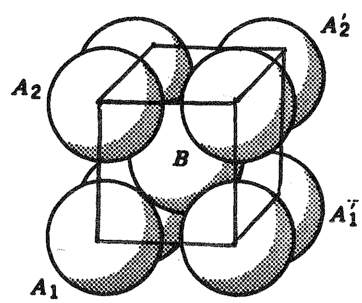
2. **C.N. of interstice of model** 8

3. **Sketch of packing along the plane $A_1A_1'A_2A_2'$**




*(b)*



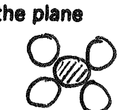




1. **Outline unit cell in model and give name of its shape**

   cube

2. **C.N. of central (shaded) sphere (*B*)** 8

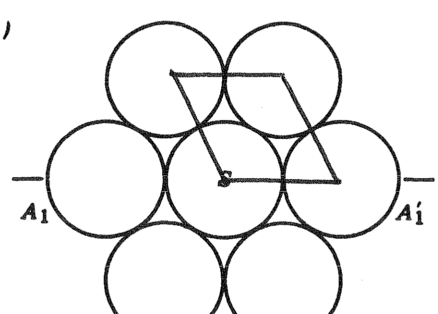
3. **Sketch of packing along the plane $A_1A_1'A_2A_2'$.**

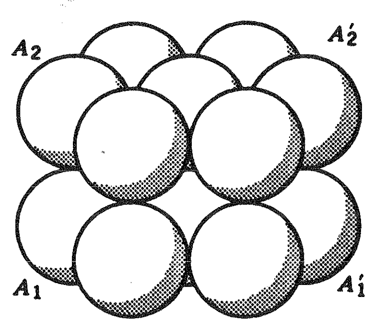


4. **What differentiates this packing from that shown in part *a*?**

   an expansion about the shaded (interstitial) sphere (B)

*(c)*



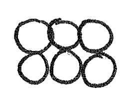




1. **Outline smallest unit cell choice in plan view and give name of its shape**

   rhombus

2. **C.N. of sphere *S* in the two–layer sequence** 7

3. **Sketch of packing along $A_1A_2A_1'A_2'$**



4. **After adding a third layer below the plane $A_1A_1'$, what becomes of the C.N. of sphere *S*?** 8

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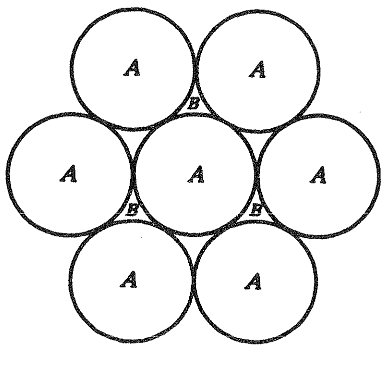
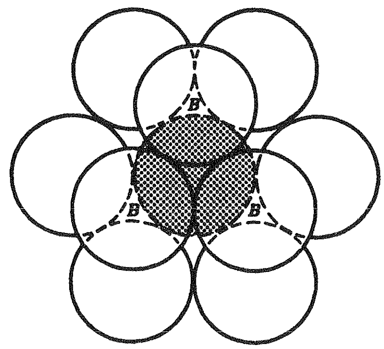
**FIGURE 3.4** *(continued)*

***(d)***



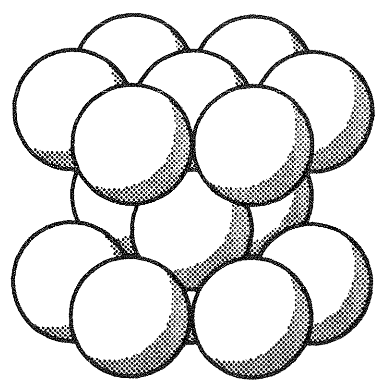

One layer of spheres;
***B*** is the location of voids




Two-layer stacking ***AB***

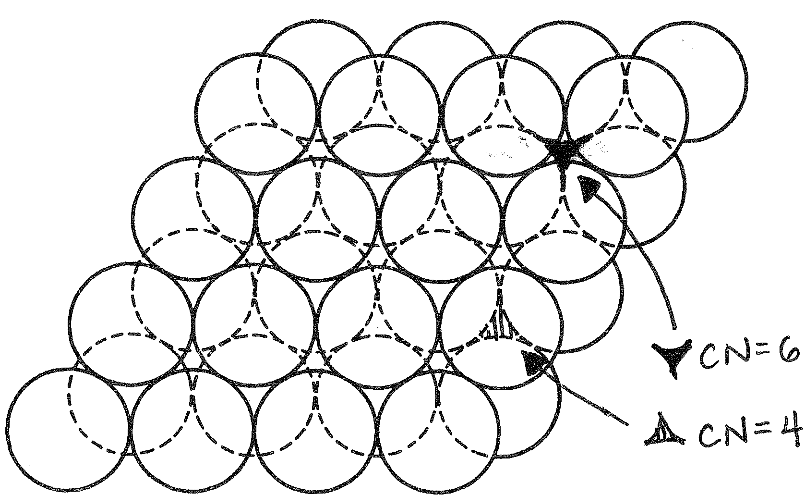
C.N. of shaded sphere is 9

In three-layer stacking ***ABA*** the C.N. of any sphere is 12



Three-layer stacking ***ABA***
(hexagonal close-packed)

***(e)***




1. Give stacking sequence of this two-layer stack (using ***A*** and ***B*** notation)
   ABABAB...

2. This stacking has two different types of interstices with different coordination numbers. Locate these two types throughout the drawing and give their C.N.:
   ________

# EXERCISE 3

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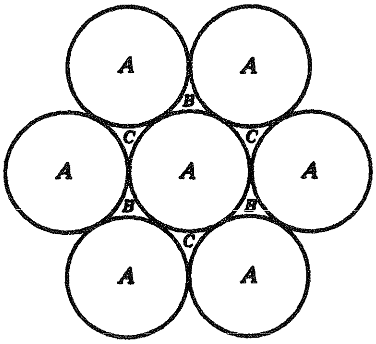
**FIGURE 3.4** *(continued)*

*(f)*



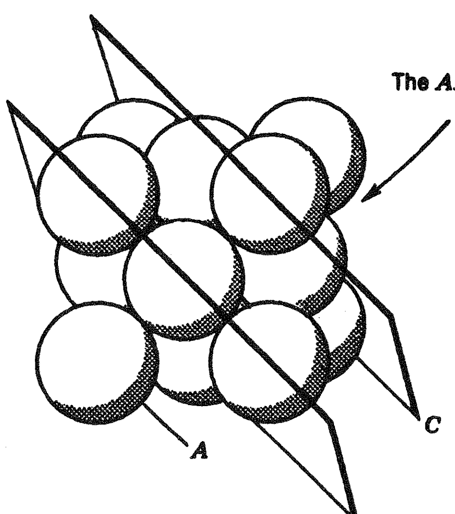

One layer of spheres with all void spaces identified

 ***B*** **voids**

 ***C*** **voids**

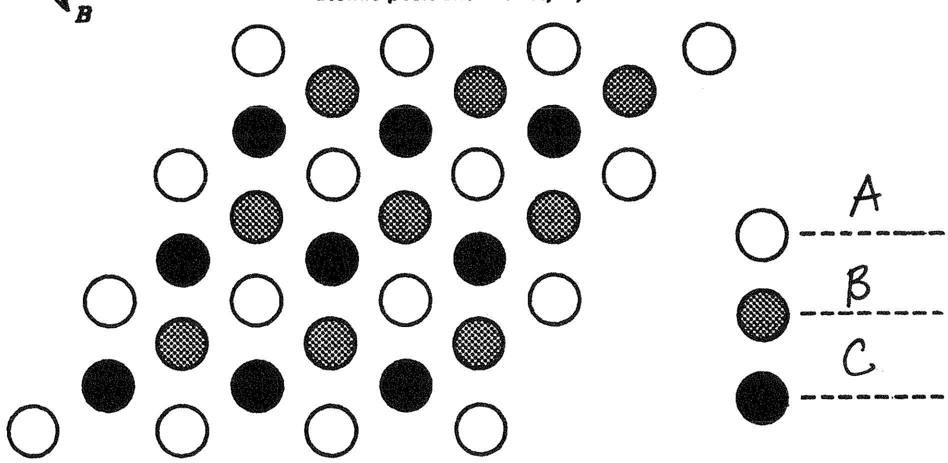
**Instead of stacking a sequence of *AB AB AB*. . . . (as in Fig. 3.4*d*), we can stack a somewhat different sequence *ABC ABC*. . . . .**

**What is the C.N. of any sphere in such a sequence?** 12




**The *ABC ABC* sequence is known as cubic close-packed.**

**In the schematic projection of such a sequence, label the atomic positions with *A*, *B*, and *C*.**



# EXERCISE 3

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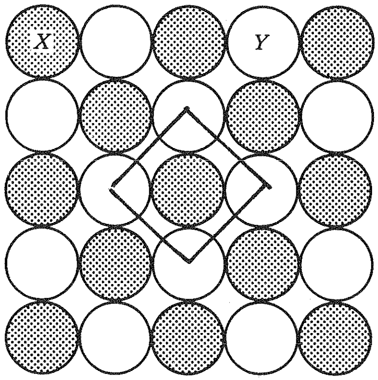
**FIGURE 3.5** Assignment on the two-dimensional packing of two types of equal-sized spheres.

**In each of these four drawings outline an appropriate unit cell* and determine the composition of this unit cell (e.g., $XY_2$, etc.).**

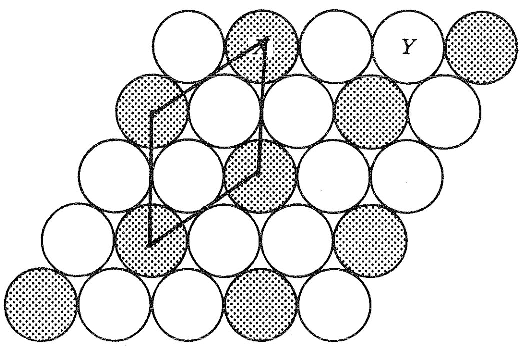
***A unit cell is the smallest unit of repeat in a pattern; it will yield the entire pattern when trannslated repeatedly without rotation**

*(a)*



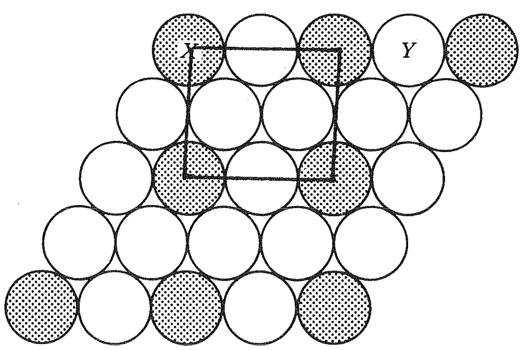

$X_1 Y_1$

*(b)*



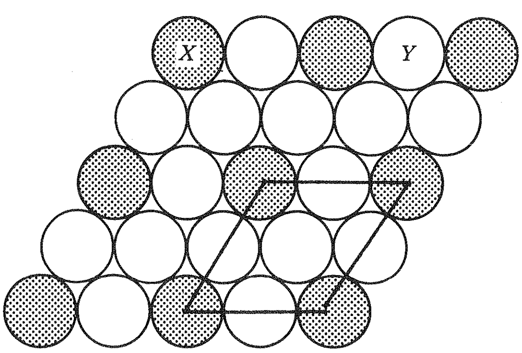

$X_1 Y_2$

*(c)*




$X_1 Y_3$

*(d)*




$X_1 Y_3$

**Single layers of equally-sized spheres (= atoms)**

# EXERCISE 3

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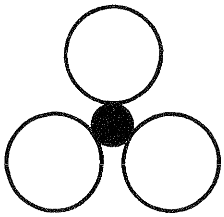
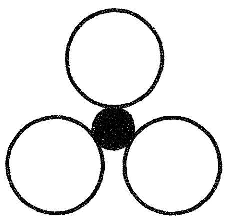
**FIGURE 3.6** Assignment on the calculation of average bond strengths.



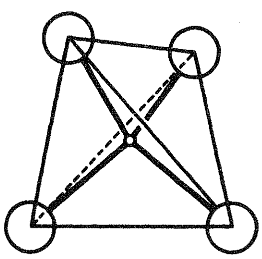
Average bond strength, or e.v. = 1 1/3

Triangular: $CO_3$ with $C^{4+}$ and $O^{2-}$



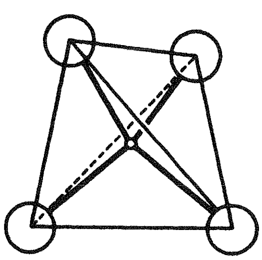
e.v. = 1.0

Triangular: $BO_3$ with $B^{3+}$ and $O^{2-}$



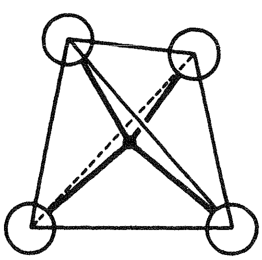
e.v. = 1 1/2

Tetrahedral: $SO_4$ with $S^{6+}$ and $O^{2-}$



e.v. = 1 1/4

Tetrahedral: $PO_4$ with $P^{5+}$ and $O^{2-}$



e.v. = 1.0

Tetrahedral: $SiO_4$ with $Si^{4+}$ and $O^{2-}$

# EXERCISE 3

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*TABLE 3.2* Assignment on the Calculation of the Radius Ratios for Various Compounds.

| *Compound* | *Radius Ratio* $R_X : R_Z$ *(Radii Given Below)* | *Predicted Coordination Number*[a] (C.N.) |
|---|---|---|
| ZnS | 0.40 | 4 |
| $SiO_2$ | 0.30 | 4 |
| $Al_2O_3$ | 0.36 | 4 |
| $Fe_2O_3$ | 0.46 | 6 |
| FeO | 0.53 | 6 |
| CaO | 0.71 | 6 |
| MgO | 0.47 | 6 |
| $TiO_2$ | 0.49 | 6 |
| NaCl | 0.54 | 6 |
| $CaF_2$ | 0.74 | 8 |
| CsCl | 0.92 | 8 |
| CuCu (metal) | 1 | 12 |

$Zn^{2+}$[6] = 0.74 Å; $S^{2-}$[4] = 1.84 Å; $O^{2-}$[3] = 1.36Å; $Si^{4+}$[4] = 0.26 Å; $Al^{3+}$[4] = 0.39Å; $Fe^{3+}$[6] = 0.65Å; $Fe^{2+}$[6] = 0.78Å; $Ca^{2+}$[6] = 1.00Å; $Mg^{2+}$[6] = 0.72Å; $Ti^{4+}$[6] = 0.61Å; $Na^{+}$[6] = 1.02Å; $Cl^{-}$[6] = 1.81Å; $F^{-}$[6] = 1.33Å; $Cs^{+}$[6] = 1.67Å; Cu(atomic) = 1.28Å; ionic and atomic radii taken from Tables 3.7 and 3.8, respectively, in *Manual of Mineral Science*, 23rd ed., p. 47 and p. 49. Numbers inside square bracket are coordination numbers.

[a] Predicted coordination numbers may not equal the coordination number in the actual crystal structure. This is in large part because in real structures the atoms and ions do not behave as perfect spheres. Indeed ions and atoms, especially large ones, are easily *polarized*, which means that their shape has become somewhat ellipsoidal, instead of being truly spherical.