

(Wave Function) Ψ

$\Psi(R, \Theta, \Phi)$

$\Psi(x, y, z)$:

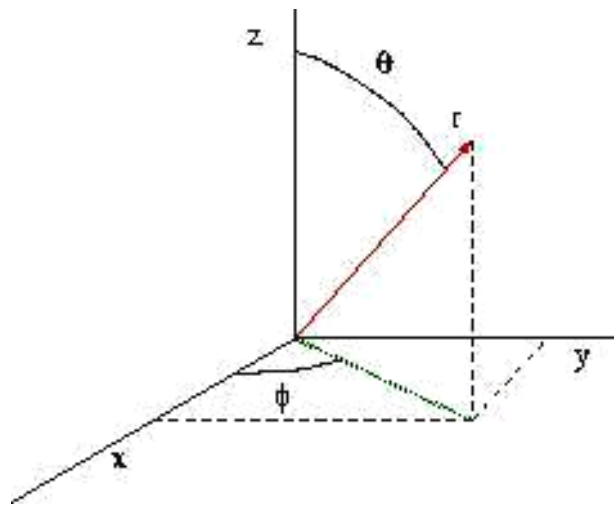
$$: \quad : \quad \Psi \quad .1$$

$$R$$

$$(\Theta, \Phi) \quad .2$$

$\Theta \quad \Phi$

$$\Psi(R, Y) : \quad \Psi \quad (Y)$$



$$\Psi(R, \Theta, \Phi) = \Psi(R, Y)$$

(1)

:(The Radial Function)

$$(l) \quad (n) \quad : \quad R$$

(Bohr)

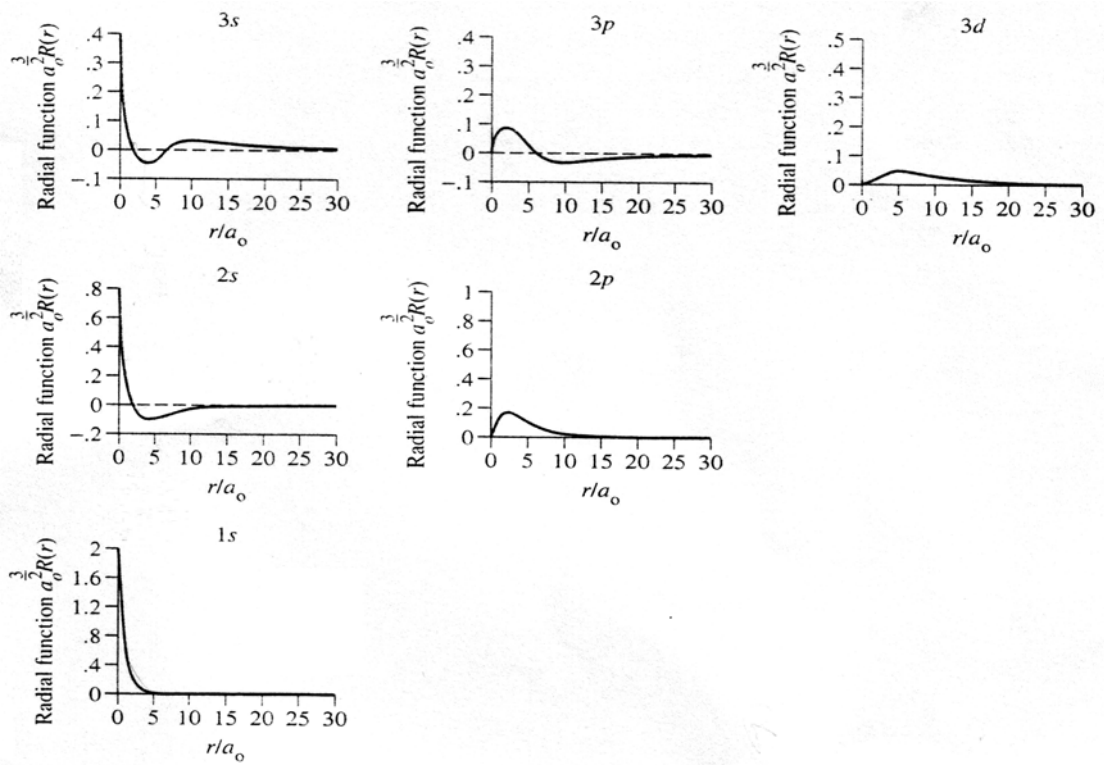
$$(1 = n$$

:

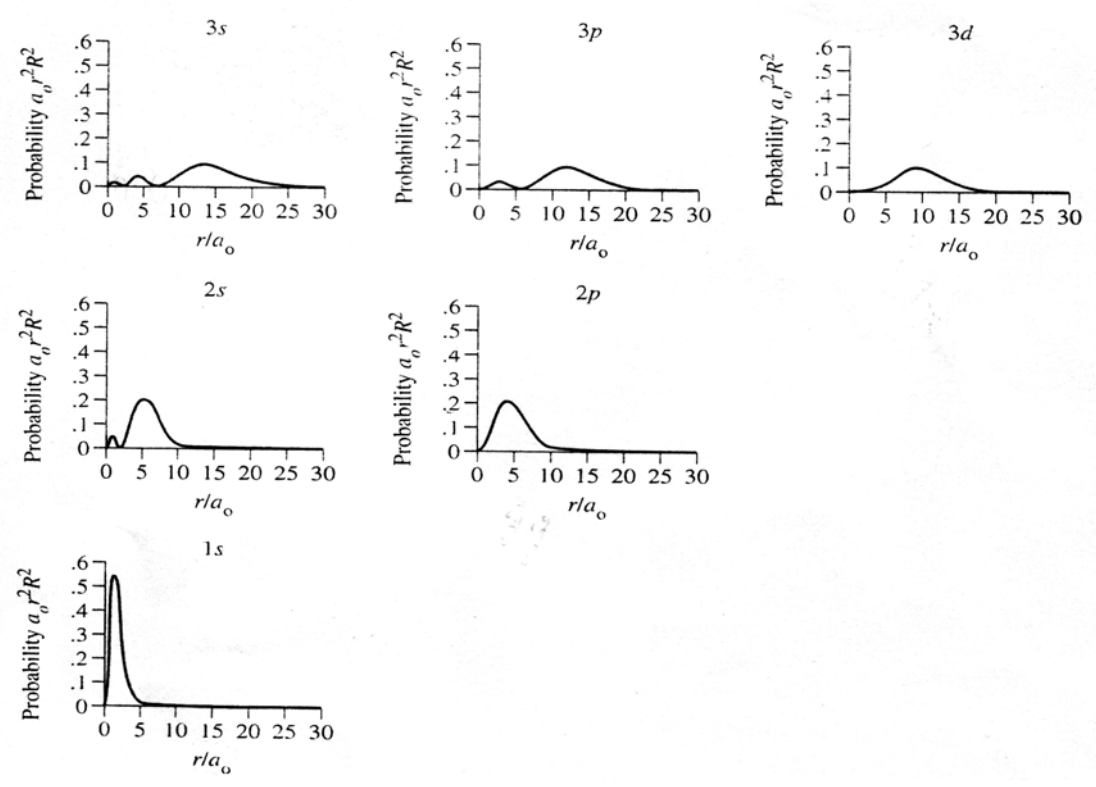
$$a_0 = 52.9 \text{ Pm}$$

$$= 52.9 \times 10^{-12} \text{ m}$$

:The Radial Probability Function (R^2)



Radial Wave Functions



(2)

R^2

R

$n = 1, 2, 3$

1s

3d

$$r = 5 a_0$$

$$r = 20 a_0$$

$$r = 9 a_0$$

$$r = 0$$

s

:(The Angular Function)

R

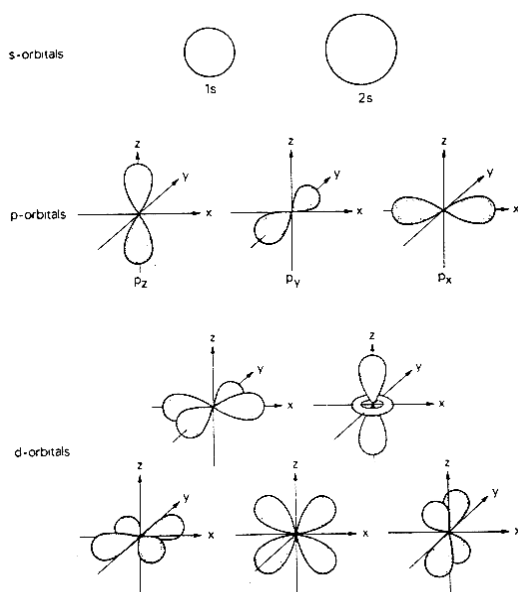
Y

Y

Y

$$m_l \quad l$$

.s , p , d



(3)

(Nodal Surface)

$$) \quad 2s \quad (2)$$

$$r = 2 a_0 \quad ($$

Ψ

$$\Psi \quad (\Psi^2)$$

:

$$\Psi(R, \Theta, \Phi) = \Psi(R, Y)$$

$$. \quad 0 = Y \quad 0 = R$$

Ψ

:(Spherical Nodes)

(Radial Nodes)

$$(n - l - 1)$$

$$0 = R$$

$$l = 0 \quad n = 1 \quad 1s$$

$$1s \quad 0 = 1 - 0 - 1$$

$$n = 4, l = 0 \quad 4s$$

$$4s \quad 3 = 4 - 0 - 1 =$$

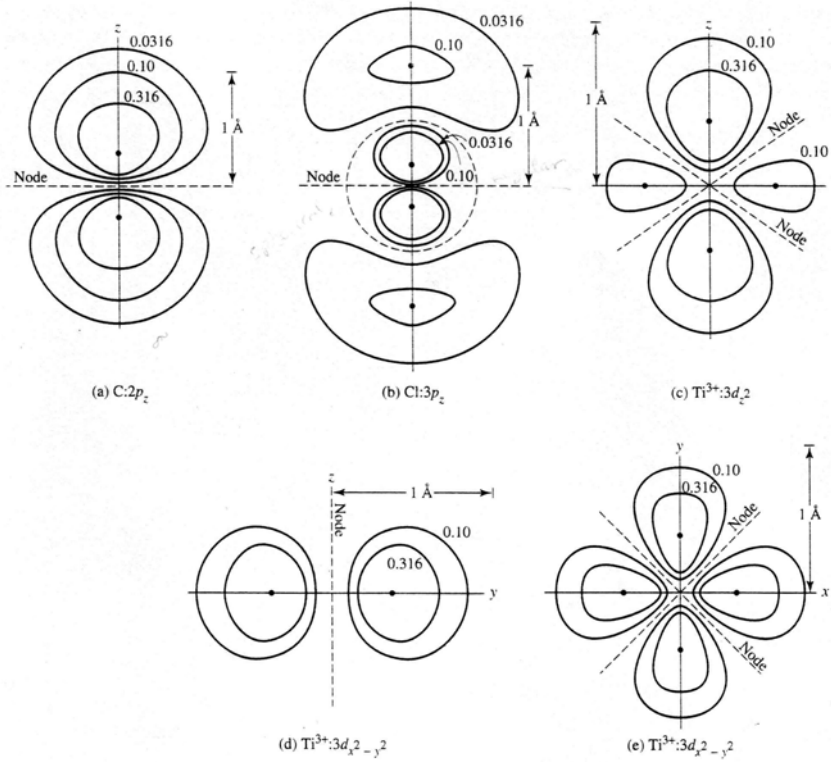
$$n = 4, l = 2 \quad 4d$$

$$4 - 2 - 1 = 1 =$$

:(Angular Nods)

$$. \quad \Phi \quad \Theta$$

$$0 = Y$$



(4)

.6 1 p

| Number of electrons | Arrangement | Unpaired e ⁻ | Multiplicity |
|---------------------|--------------|-------------------------|--------------|
| 1 | ↑ — — | 1 | 2 |
| 2 | ↑ ↑ — | 2 | 3 |
| 3 | ↑ ↑ ↑ | 3 | 4 |
| 4 | ↑↓ ↑ ↑ | 2 | 3 |
| 5 | ↑↓ ↑↓ ↑ | 1 | 2 |
| 6 | ↑↓ ↑↓ ↑↓ | 0 | 1 |

(6)

:(Coulombic energy of repulsion IIc)

:(Exchange Energy IIe)

.1s² 2s² 2p²

.2p

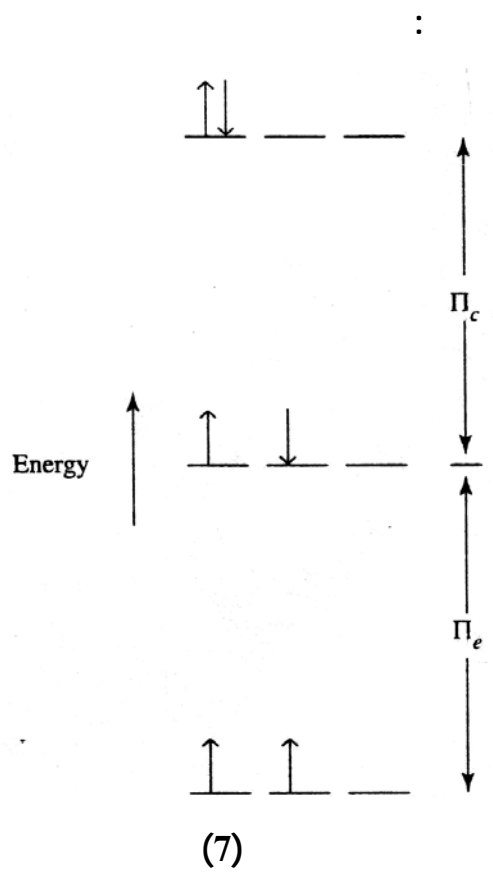
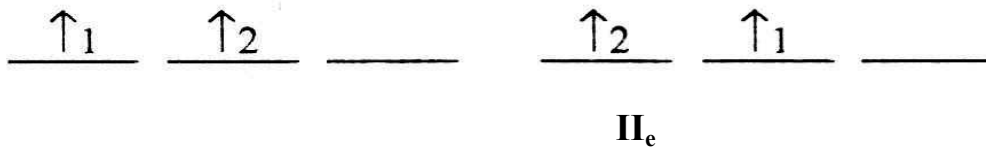
(1) ↑↓ — — (2) ↑ ↓ — (3) ↑ ↑ —

) II_c

(

II_c

. - +

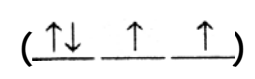
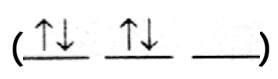


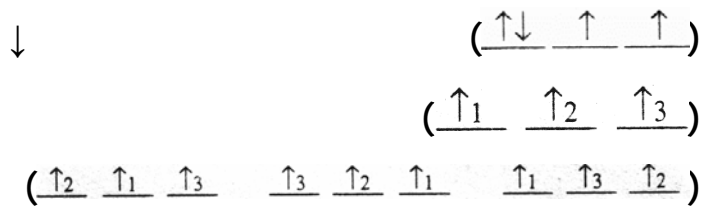
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$$\Pi = \Pi_e + \Pi_c$$

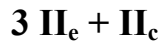
Π_c
 Π_e

p

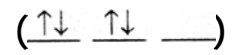




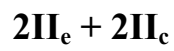
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:



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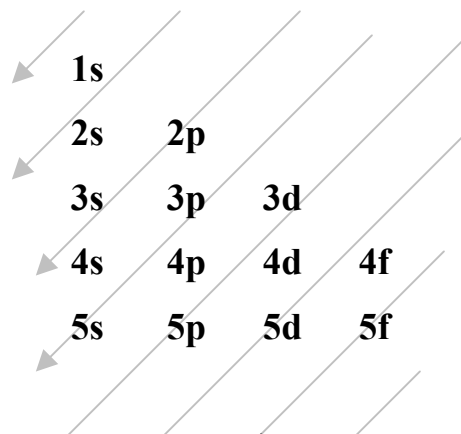


Π_e

Π_c

(Shielding)

4s 4d 5s 3d 4s 6d 5f 5d 4f 5d



)

Z^*

Z

:

(

$$Z^* = Z - S$$

S

:

.1

(1s) (2s, 2p) (3s, 3p) (3d) (4s, 4p) (4d) (4f) (5s, 5p) (5d) (5f)

()

: np ns

.2

0,35

0,85 (n - 1)

(n - 2)

1

:

nf nd

.3

.0,35 nf nd

nf nd

:

.1s² 2s² 2p⁴

1s

S = 0,35

$$\therefore Z^* = Z - S$$

$$\therefore Z^* = 8 - 0,35 = 7,65$$

.(n)

5 (n - 1)

) 2s

$$S = 2 \times (0,85) - 5 \times (0,35) = 3,45$$

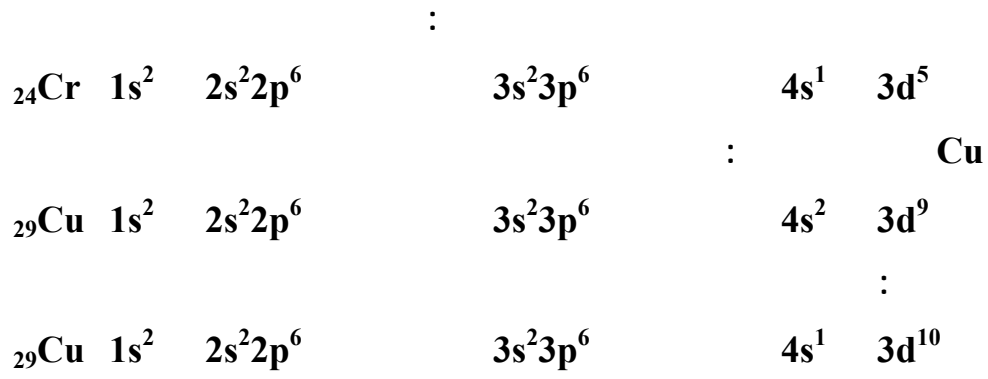
$$Z^* = 8 - 3,45 = 4,55$$

:

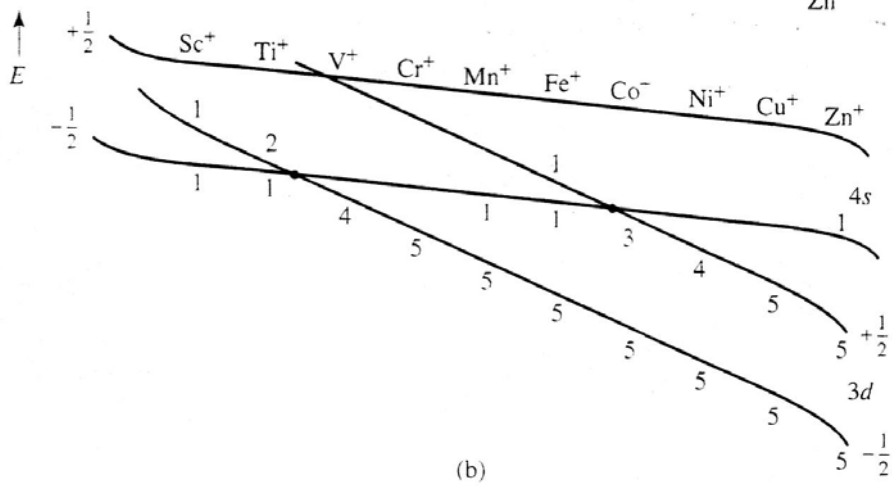
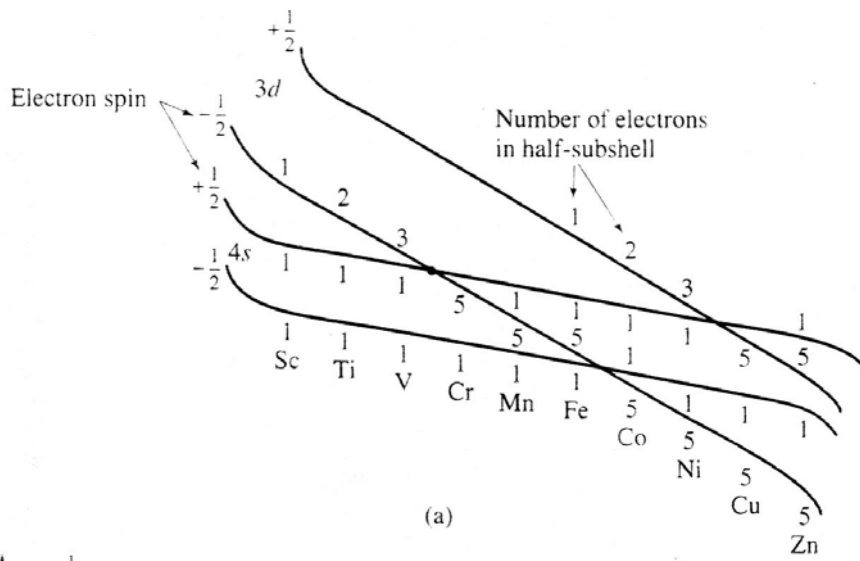
²⁴Cr 1s² 2s²2p⁶

3s²3p⁶

4s² 3d⁴



d



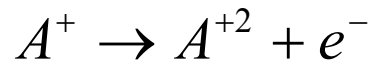
(8)

(Ionization Energy)

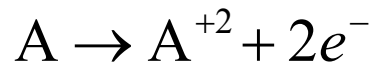
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.1st IE



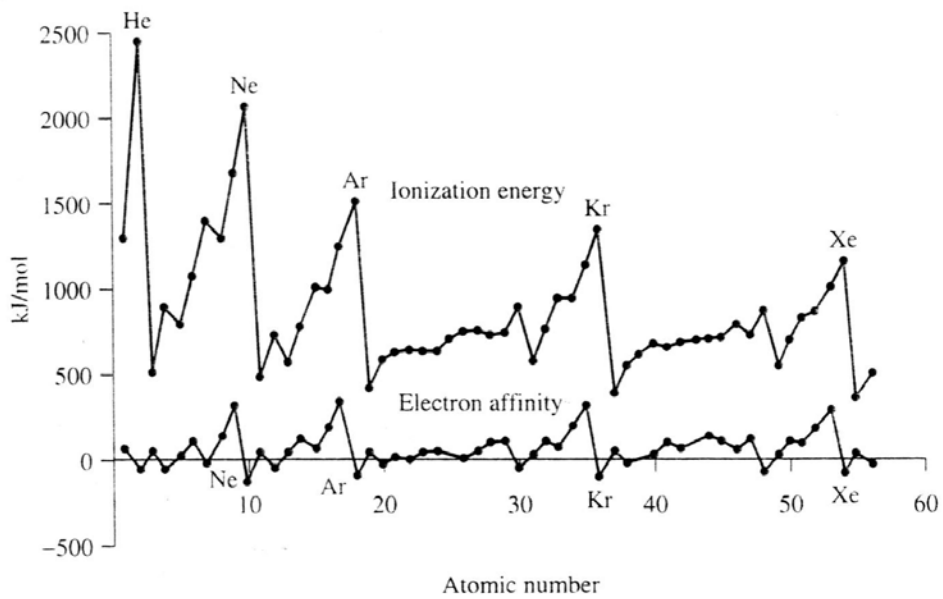
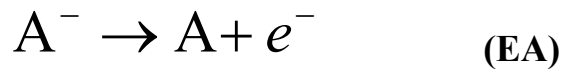
.2nd IE



.1st + 2nd IE

(Electron Affinity)

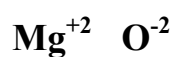
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(9)

Iso-electronic ions

10



| <i>Ion</i> | <i>Protons</i> | <i>Electrons</i> | <i>Radius (pm)</i> |
|------------------|----------------|------------------|--------------------|
| O^{2-} | 8 | 10 | 126 |
| F^{-} | 9 | 10 | 119 |
| Na^{+} | 11 | 10 | 116 |
| Mg^{2+} | 12 | 10 | 86 |

TABLE 2-10
Ionic radius and total number of electrons

| <i>Ion</i> | <i>Protons</i> | <i>Electrons</i> | <i>Radius (pm)</i> |
|------------------|----------------|------------------|--------------------|
| O^{2-} | 8 | 10 | 126 |
| S^{2-} | 16 | 18 | 170 |
| Se^{2-} | 34 | 36 | 184 |
| Te^{2-} | 52 | 54 | 207 |

TABLE 2-11
Ionic radius and ionic charge

| <i>Ion</i> | <i>Protons</i> | <i>Electrons</i> | <i>Radius (pm)</i> |
|------------------|----------------|------------------|--------------------|
| Ti^{2+} | 22 | 20 | 100 |
| Ti^{3+} | 22 | 19 | 81 |
| Ti^{4+} | 22 | 18 | 75 |