(ACTC) ADVANCE	ED CHEMISTRY TUITION CENT	RE, 41/1 PWD ROAD, N	NAGERCOIL, 9952340892.

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3	$E_{n} = \frac{-(1312.8)Z^{2}}{2}$	It is used to calculate	If $l = 1$, $m = -1$, 0 , $+$	S values are $+^{1}/_{2}$
	$E_n = \frac{1}{n^2}$	the orbital angular	1	$(or) - \frac{1}{2}$.
	kJ mol ^{−1} .	momentum by the		
		formula $\sqrt{l(l+1)} \frac{h}{2\pi}$		Pa _s
4	It represents the	1 = 0, 1, 2, 3		14
	distance of the electron	Subshell = s , p , d , f		
	from the nucleus.	No. of electrons = 2 ,		
		6, 10, 14		
	n = 1, 2, 3, 4 K L M N			

- ➤ Hund's rule of maximum multiplicity It states that electron pairing in the degenerate orbitals does not take place until all the available orbitals contains one electron each.
- **Electronic configuration** The distribution of electrons into various orbitals of an atom is called its electronic configuration.
- **Exchange energy** During the exchanging process of two or more electrons with the same spin present in degenerate orbitals, the amount of energy released in called exchange energy.

Quantum Mechanical Model of Atom Unit 2

Choose the best answer

1. Electronic configuration of species M²⁺ is 1s² 2s² 2p⁶ 3s² 3p⁶ 3d⁶ and its atomic weight is 56. The number of neutrons in the nucleus of species M is

a) 26

- b) 22
- c) 30

d) 24

2. The energy of light of wavelength 45 nm is

- a) 6.67×10^{15} J
- b) 6.67×10^{11} J c) 4.42×10^{-18} J

- d) 4.42×10^{-15} J
- 3. The energies E₁ and E₂ of two radiations are 25 eV and 50 eV respectively. The relation between their wavelengths ie λ_1 and λ_2 will be
- a) $\frac{\lambda_1}{\lambda_2} = 1$

- d) $2\lambda_1 = \lambda_2$

4. Splitting of spectral lines in an electric field is called

- a) Zeeman effect
- b) Shielding effect c) Compton effect
- d) Stark effect
- 5. Based on equation $E = -2.178 \times 10^{-18} J_{\frac{z^2}{n^2}}$, certain conclusions are written. Which of them is not correct ? (NEET)
- a) Equation can be used to calculate the change in energy when the electron changes orbit **b**) For n = 1, the electron has a more negative energy than it does for n = 6 which means that the electron is more loosely bound in the smallest allowed orbit
- c) The negative sign in equation simply means that the energy of electron bound to the nucleus is lower than it would be if the electrons were at the infinite distance from the nucleus.
- d) Larger the value of n, the larger is the orbit radius.

Dedication! Distinction!!! Determination!! (ACTC) ADVANCED CHEMISTRY TUITION CENTRE, 41/1 PWD ROAD, NAGERCOIL, 9952340892. (i) 3 0 $1 - \frac{1}{2}$ (ii) 2 (iii)4 $+\frac{1}{2}$ $0 -1 + \frac{1}{2}$ (iv)1 $4 \quad 3 \quad -\frac{1}{2}$ (v) 3 Page | Which of the following sets of quantum number is not possible? 16 a) (i), (ii), (iii) and (iv) **b) (ii), (iv) and (v)** c) (i) and (iii) d) (ii), (iii) and (iv) 18. How many electrons in an atom with atomic number 105 can have (n+1) = 8? a) 30 d) unpredictable 19. Electron density in the yz plane of $3d_x^2 - y^2$ orbital is d) 0.90 a) zero 20. If uncertainty in position and momentum are equal, then minimum uncertainty in velocity is a) $\frac{1}{m}\sqrt{\frac{h}{\pi}}$ b) $\sqrt{\frac{h}{\pi}}$ c) $\frac{1}{2m}\sqrt{\frac{h}{\pi}}$ d) $\frac{h}{4\pi}$ 21. A macroscopic particle of mass 100 g and moving at a velocity of 100 cm s⁻¹ will have a de a) $\frac{1}{m} \sqrt{\frac{h}{\pi}}$ Broglie wavelength of b) 6.6×10^{-30} cm c) 6.6×10^{-31} cm a) 6.6×10^{-29} cm $d)6.6 \times 10^{-32} cm$ 22. The ratio of de Broglie wavelengths of a deuterium atom to that of an α - particle, when the velocity of the former is five times greater than that of later, is c) 2.5 d) 0.4 b) 0.2 a) 4 23. The energy of an electron in the 3rd orbit of hydrogen atom is –E. The energy of an electron in the first orbit will be a) -3Ec) –E / 9 d) - 9E24. Time independent Schnodinger wave equation is b) $\nabla^2 \psi + \frac{8\pi^2 m}{h^2} (E + V) \psi = 0$ a) $\hat{H}\psi = E\psi$ c) $\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} + \frac{2m}{h^2} (E - V) \psi = 0$ d) all of these 25. Which of the following does not represent the mathematical expression for the Heisenberg uncertainty principle? b) Δx . $\Delta v \ge \frac{h}{4\pi m}$ c) ΔE . $\Delta t \ge \frac{h}{4\pi}$ d) ΔE . $\Delta x \ge \frac{h}{4\pi}$ a) $\Delta x \cdot \Delta p \geq \frac{h}{4\pi}$ Answer the following 26. Which quantum number reveal information about the shape, energy, orientation

and size of orbitals?

Magnetic quantum number

	Quantum Number	Information Obtained
(i)	Principal Quantum no.	Size and energy
(ii)	Azimuthal Quantum no.	Shape
(iii)	Magnetic Quantum no.	Orientation

27. How many orbitals are possible for n = 4?

n = 4, 1 = 0, 1, 2, 3 four sub-shells => s, p, d, f

1 = 0 $m_1 = 0$; one 4s orbital

 $1 = 1 \text{ m}_1 = -1, 0, +1$; three 4p orbitals.

 $1 = 2 \text{ m}_1 = -2, -1, 0, +1, +2$; five 4d orbitals.

 $1 = 3 \text{ m}_1 = -3, -2, -1, 0, +1, +2, +3$; seven 4f orbitals Over all sixteen orbitals.

(Or)
$$n^2 = 4^2 = 16$$

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28. How many radial nodes for 2s, 4p, 5d and 4f orbitals exhibit? How many angular nodes?

Orbital	N	1	Radial node n-l-1	Angular node l
2s	2	0	1	0
4p	4	1	2	1
5d	5	2	2	2
4f	4	3	0	3

29. The stabilization of a half filled d- orbital is more pronounced than that of the porbital why?

- (i) The half filled d- orbital is much stabilized than the p-orbital.
- (ii) This is due to its high exchange energy and symmetry than that of p-orbital.
 - 30. Consider the following electronic arrangements for the d⁵ configuration.

41	41	_	
11	11	1	

1	1	1	41	
ı		- I _№ I		
		_		

1	1	1	1	1

(a)

(b)

(c)

- (i) which of these represents the ground state
- (ii) which configuration has the maximum exchange energy.
- (i) C) Ground state
- (ii) c) Maximum exchange energy:

1 1	1 1	1 1	1 1	1 1
1 .	1 .	1 .	1 .	

31. State and explain pauli's exclusion principle

"No two electrons in an atom can have the same set of values of all four quantum number".

For the lone electron present in hydrogen atom, the four quantum numbers are: n = 1; l = 0; m = 0 and s = +1/2. For the two electrons present in **Helium**, $1s^2$

		1	,	
	N	1	m	S
First electron	1	0	0	+1/2
Second electron	1	0	0	-1/2

Spin quantum number can have only two values +1/2 and -1/2, only two electrons can be accommodated in a given orbital in accordance with pauli exclusion principle.

32. Define orbital? What are the n and l values for $3p_x$ and $4d_{x2-v2}$ electron?

An orbital is the region of space around the nucleus within the probability of finding an electron of given energy is maximum.

Orbital	n	1
$3p_x$	3	1
$4d_{x2-y2}$	4	2

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33. Explain briefly the time independent Schrödinger wave equation?

Erwin Schrodinger expressed the wave nature of electron in terms of a differential equation. This equation determines the change of wave function in space depending on the field of force in which the electron moves. The time independent Schrodinger equation can be expressed as, $\hat{H}\psi = E\psi$

Where \hat{H} is called Hamiltonian operator, ψ is the wave function and is a function of position co-ordinates of the particle and is denoted as $\psi(x, y, z)$ E is the energy of the system

$$\hat{H} = \left[\frac{-h^2}{8\pi^2 m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + V \right]$$
Can be written as,
$$\left[\frac{-h^2}{8\pi^2 m} \left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right) + V \psi \right] = E \psi$$

Multiply by $-\frac{8\pi^2 m}{h^2}$ and rearranging

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} + \frac{8\pi^2 m}{h^2} (E - V) \psi = 0$$

The above Schrödinger wave equation does not contain time as a variable and is referred to as time independent Schrödinger wave equation. This equation can be solved only for certain values of E, the total energy. i.e. the energy of the system quantised. The permitted total energy values are called Eigen values and corresponding wave functions represent the atomic orbitals.

34. Calculate the uncertainty in position of an electron, if $\Delta v = 0.1\%$ and $v = 2.2 \times 10^6$ ms⁻¹

$$\Delta x. \ \Delta p \ge \frac{h}{4\pi}$$

$$\Delta x. \ \Delta v.m = \frac{h}{4\pi}$$

$$\Delta \mathbf{X} = \frac{n}{4\pi\Delta \mathbf{v}.\mathbf{m}}$$

$$\Delta X = \frac{6.626 \times 10^{-34} \, Kgm^2 s^{-1}}{4x3.14x \, 9.1 \times 10^{-31} \, Kg \times 2.2 \times 10^3 ms^{-1}}$$

$$\Delta X = \frac{6.626 \times 10^{-34} \, x \, 10^{-3} \times 10^{31}}{4x^{-1} \, 10^{-34} \, x \, 10^{-3} \times 10^{31}}$$

$$\Delta X = \frac{6.626 \times 10^{-6}}{251.45}$$

$$\Delta x = 0.02635 \times 10^{-6}$$

$$\Delta x = 2.635 \times 10^{-8} \text{ m}$$

$$\Delta x. \Delta p \geq \frac{h}{4\pi}$$

$$\Delta x. \ \Delta p \ge 5.28 \times 10^{-35} \ \text{Kgm}^2 \text{s}^{-1}$$

$$\Delta x. (m\Delta v) \ge 5.28 \times 10^{-35} \text{ Kgm}^2 \text{s}^{-1}$$

Given
$$\Delta v = 0.1\%$$

$$v = 2.2 \times 10^6 \text{ ms}^{-1}$$
; m= $9.1 \times 10^{-31} \text{ Kg}$

$$\Delta v = \frac{0.1}{100} \times 2.2 \times 10^6 \,\text{ms}^{-1} = 2.2 \times 10^3 \,\text{ms}^{-1}$$

$$\Delta X \geq \frac{5.28 \times 10^{-35} \, Kgm^2 s^{-1}}{9.1 \times 10^{-31} \, Kg \times 2.2 \times 10^3 ms^{-1}}$$

$$\Delta x \geq 2.64 \times 10^{-8} \text{ m}$$

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35. Determine the values of all the four quantum numbers of the 8th electron in O- atom a 15th electron in the Cl atom and the last electron in chromium.

Electronic configuration of oxygen (Z=8)= $1s^2 2s^2 2p_x^2 2p_y^1 2p_z^1$

8th electron present in 2p_x orbital and an the quantum numbers are

n = principal quantum number = 2

l= azimuthal quantum number= 1

 m_1 =magnetic quantum number = either +1 or -1

 $m_s = +1/2$

Electronic configuration of chlorine (Z=17) = $1s^2 2s^2 2p^6 3s^2 3p_x^2 3p_y$

 $1s^2$

 $2p^6$

 $3s^2$

 $3p_x$ $3p_y$ $3p_z$

15th electron present in **3p_z orbital** and

the quantum numbers are n = 3, 1 = 1 $m_1 = either + 1$ or -1 and $m_s = +1/2$

Electronic configuration of chromium (Z=24) = $1s^2 2s^2 2p^6 3s^2 3p^6 3d^5 4s^1$

n=3 l=2, m=+2 s=+1/2

36. The quantum mechanical treatment of the hydrogen atom gives the energy value: E_n = $\frac{-13.6}{n^2}$ ev atom⁻¹

(i) use this expression to find ΔE between n=3 and m=4

(ii) Calculate the wavelength corresponding to the above transition

$$E_n = \frac{-13.6}{n^2} \text{ eV atom}^{-1}$$

$$n^2$$
 -13.6 -1

n = 3
$$E_3 = \frac{-13.6}{3^2} = \frac{-13.6}{9} = -1.51 \text{ eV atom}^{-1}$$

n = 4 $E_4 = \frac{-13.6}{4^2} = \frac{-13.6}{16} = -0.85 \text{ eV atom}^{-1}$

$$n = 4$$

$$E_4 = \frac{-13.6}{4^2} = \frac{-13.6}{16}$$

$$= -0.85 \text{ eV atom}^{-1}$$

$$\Delta E = (E_4 - E_3)$$

$$= (-0.85) - (-1.51) \text{ eV atom}^{-1}$$

$$= (-0.85 + 1.51)$$

=
$$0.66 \text{ eV atom}^{-1}$$
 $(1\text{eV} = 1.6 \times 10^{-19} \text{ J})$

$$\Delta E = 0.66 \times 1.6 \times 10^{-19} \,\mathrm{J}$$

$$\Delta E = 1.06 \times 10^{-19} \,\mathrm{J}$$

hv =
$$1.06 \times 10^{-19} \,\text{J} \frac{hc}{\lambda} = 1.06 \times 10^{-19} \,\text{J}$$

$$\lambda = \frac{hc}{1.06 \times 10^{-19} J} = \frac{6.626 \times 10^{-34} JS \times 3 \times 10^8 ms^{-1}}{1.06 \times 10^{-19} J}$$

$$\lambda = 1.875 \times 10^{-6} \,\mathrm{m}$$

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37.how fast must a54g tennis ball in order to have a de Broglie wavelength that is equal to that a photon of green light 5400Å?

De Broglie wavelength of the tennis ball equal to 5400 Å

$$m = 54 g$$
; $v = ?$ $\lambda = \frac{h}{mV}$ $V = \frac{h}{m\lambda}$

$$V = \frac{6.626 \times 10^{-34} JS}{54 \times 10^{-3} Kg \times 5400 \times 10^{-10} m} \quad V = 2.27 \times 10^{-26} \text{ ms}^{-1}$$

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38. For each of the following, give the sub level designation, the allowable m values and the number of orbitals (i) n=4, l=2 (ii) n=5, l=3 (iii) n=7, l=0

N	l	Sub Energy levels	m 1 values	Number of orbitals
4	2	4d	-2, -1, 0,+1,+2	Five 4d orbitals
5	3	5f	-3,-2, -1, 0, +1,+2, +3	Seven 5f orbitals
7	0	7s	0	One 7s orbitals

39. Give the electronic configuration of Mn²⁺ an Cr³⁺

Ions	No. of electrons	Electronic configuration
Mn ²⁺	23	$1s^2$, $2s^2$, $2p^6$, $3s^2$, $3p^6$, $3d^5$
Cr ³⁺	21	1s ² , 2s ² , 2p ⁶ , 3s ² , 3p ⁶ , 3d ³

40. Describe the Aufbau principle

The word Aufbau in German means 'building up'.

- In the ground state of the atoms, the orbitals are filled in the order of their increasing energies.
- That is the electrons first occupy the lowest energy orbitals available to them.
- Once the lower energy orbitals are completely filled, then the electrons enter the next higher energy orbitals.
- The order of filling of various orbitals as per Aufbau principle is

For example: Electronic configuration of chromium (Z=24) = $1s^2 2s^2 2p^6 3s^2 3p^6 3d^5 4s^1$

41. An atom of an element contains 35 electrons and 45 neutrons. Deduce

- (i) the number of protons
 - (ii) the electronic configuration for the element
 - (iii) All the four quantum numbers for the last electron

Ans. (i) No of protons = 35

Electronic configuration 1s², 2s², 2p⁶, 3s², 3p⁶, 4s², 3d¹⁰, 4p⁵ (ii)

(iii)

11	11	1
$4p_x$	$4p_y$	$4p_z$

Last electron present in 4P_y orbital

$$n = 4$$
, $l = 1$ $m_1 = either + 1$ or -1 and $s = -1/2$

42. Show that the circumference of the bohr's orbit for the hydrogen atom is an integral multiple of the de Broglie wave length associated with the electron revolving around the nucleus.

Ans: Quantization of angular momentum and de Broglie concept.

- According to the de Broglie concept, the electron that revolves around the nucleus electron exhibits both particle and wave character.
- In order for the electron wave to exist in phase, the circumference of the orbit should be an integral multiple of the wavelength of the wave. Otherwise, the electron electron wave is out of phase.

Circumference of the orbit = $n\lambda$

$$2\pi r = n\lambda$$

$$2\pi r = nh / mv$$

Rearranging, mvr = $nh/2\pi$ Angular momentum = $nh/2\pi$

The above equation was already predicted by Bohr. Hence, De Broglie and Bohr's concepts are in agreement with each other.

43. Calculate the energy required for the process. $He^{+}_{(g)} \rightarrow He^{2+} + e^{-}$ The ionisation energy required for the H atom in its ground state is -13.6 ev atom⁻¹.

$$He^+ \rightarrow He^{2+} + e^-$$

$$E_n = \frac{-13.6z^2}{n^2}$$
 $E_1 = \frac{-13.6(2)^2}{(1)^2} = -54.4$

$$E_{\infty} = \frac{-13.6(2)^2}{(\infty)^2} = 0$$

∴ Required Energy for the given process

$$= E_{\infty} - E_1 = 0 - (-54.4) = 54.4$$
ev.

44. An ion with the mass number 37 possesses unit negative charge. If the ion contains 11.1 % more neutrons than electrons. Find the symbol of the ion.

	Atom	Uni-negative ion
Number of electron	X-1	X
Number of protons	X-1	X - 1
Number of neutrons	Y	Y

Given that $y_1 = x + 11.1\%$ of x

$$=\left(x+\frac{11.1}{100}x\right)=x+0.111x$$

$$y = 1.111 x$$

Mass number = 37

Number of protons number of neutrons = 37

$$(x-1) + 1.111 x = 37$$

$$X + 1.111x = 38$$

2.111 x = 38 x =
$$\frac{38}{2.11}$$
; x = 18.009

$$x = 18$$
 (whole number)

 $\therefore \text{ Atomic number} = x - 1 = 18 - 1 = 17$

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Mass number = 37

Symbol of the ion ³⁷₁₇Cl

45. The Li ion is a hydrogen like ion that can be described by the Bohr's model. Calculated the Bohr radius of the third orbit and calculate the energy of the electron in 4th orbit

$$r_n = \frac{(0.529)n^2}{z} A$$
 $E_n = \frac{-13.6 (z^2)}{n^2} \text{ ev atom}^{-1}$

for $Li^{2+} Z = 3$

Bohr radius for the third orbit (r_3)

$$= \frac{(0.529)(3)^2}{3} = 0.529 \times 3 = 1.587 \text{ Å}$$

Energy of an electron in the fourth orbit

$$(E_4) = \frac{-13.6(3)^2}{(4^2)} = -7.65 \text{ eV atom}^{-1}$$

46. Protons can be accelerated in particle accelerators. Calculate the wavelength (in Å) of such accelerated proton moving at $2.85 \times 10^8 \text{ms}^{-1}$

(the mass of proton is 1.673×10^{-27} Kg)

$$V = 2.85 \times 10^{8} \text{ ms}^{-1}; \quad m_{p} = 1.673 \times 10^{-27} \text{ Kg}$$

$$\lambda = \frac{h}{mv} \qquad = \frac{6.626 \times 10^{-34} \text{ kgm}^{2} \text{ms}^{-1}}{1.673 \times 10^{-27} kg \times 2.85 \times 10^{8} \text{ ms}^{-1}} \qquad = 1.389 \times 10^{-15} \text{m} \quad [\text{ Å} = 10^{-10} \text{m}]$$

$$\rightarrow$$
 $\lambda = 1.389 \times 10^{-5} \text{ Å}$

47. What is the de Broglie wave length(in cm) of a 160g cricket ball travelling at 140 Km hr⁻¹.

m = 160g = 160 × 10⁻³ kg
v = 140 Km hr⁻¹ =
$$\frac{140 \times 10^3}{60 \times 60}$$
 ms⁻¹
v = 38.88ms⁻¹
 $\lambda = \frac{h}{mv} = \frac{6.626 \times 10^{-34} \text{ kgm}^2 \text{ms}^{-1}}{160 \times 10^{-3} kg \times 38.88 \text{ ms}^{-1}}$
 $\lambda = 1.065 \times 10^{-34} \text{m}$

wave length in cm =1.065 x 10^{-34} x 100 =1.065 x 10^{-32} cm

48. Suppose that the uncertainty in determining the position of an electron in an orbit is 0.6Å. what is the uncertainty in its momentum?

$$\Delta x = 0.6 \text{Å} = 0.6 \times 10^{-10} \text{m}$$

$$\Delta p = ?; \qquad \Delta x \cdot \Delta p \ge \frac{h}{4\pi}$$

$$\Delta x \cdot \Delta p \ge 5.28 \times 10^{-35} \text{ kgm}^2 \text{s}^{-1}$$

$$(0.6 \times 10^{-10}) \cdot \Delta p \ge 5.28 \times 10^{-35} \text{ kgm}^2 \text{s}^{-1}$$

$$\Delta p \ge \frac{5.28 \times 10^{-35} \text{ kgm}^2 \text{s}^{-1}}{0.6510^{-10} \text{m}}$$

$$\Delta p \ge 8.8 \times 10^{-25} \text{ kgm s}^{-1}$$

49. Show that if the measurement of the uncertainty in the location of the particle is is equal to its de Broglie wavelength, the minimum uncertainty in its velocity/ 4π .

$$\Delta \mathbf{x} = \Delta \mathbf{v} = ? \qquad \Delta \mathbf{x} \cdot \Delta \mathbf{p} \ge \frac{h}{4\pi} \qquad \lambda (\mathbf{m} \ \Delta \mathbf{v}) \ge \frac{h}{4\pi}$$

$$\Delta \mathbf{v} \ge \frac{h}{4\pi \ (m\lambda)} \ \Delta \mathbf{v} \ge \frac{h}{4\pi \ \times m \ \times \frac{h}{mv}} \quad [\lambda = \frac{h}{mv}] \ \Delta \mathbf{v} \ge \frac{v}{4\pi} \quad ;$$

Therefore, minimum uncertainty in velocity = $\frac{v}{4\pi}$

50. What is the de Broglie wavelength of an electron, which is accelerated from the rest. through a potential difference of 100V?

Potential difference =
$$100\text{V}$$

= $100 \times 1.6 \times 10^{-19}\text{J}$

$$\lambda = \frac{h}{\sqrt{2mev}} = \frac{6.626 \times 10^{-34} \text{ kgm}^2 \text{ms}^{-1}}{\sqrt{2 \times 9.1 \times 10^{-31} \text{ Kg} \times 100 \times 1.6 \times 10^{-19} \text{J}}}$$

$$\lambda = 1.22 \times 10^{-10}\text{m}$$

51. Identify the missing quantum numbers and the sub energy level

n	1	m	Sub energy level
?	?	0	4d
3	1	0	?
?	?	?	5p
?	?	-2	3d

Answer:

n	1	M	Sub energy level
4	2	0	4d
3	1	0	3p
5	1	Any one value $-1, 0, +1$	5p
3	2	-2	3d