Term symbols ppt

Atomic Term Symbols • The stationary states of multi-electron atom are determined by the general characteristics of Atom, not those of the individual electrons contained in the atom. • What are these general characteristics? • The total orbital angular momentum of the electrons, L • The total spin angular momentum of the electrons, S • The total angular momentum of the atom, J • Thus, the eigenstates of Hamiltonian for the atom are marked by these properties. These labels are called • Atomic Term Symbols.Atomic Term Symbols • The definition of the term symbol: • 2S +1LJ • Note: In the symbol, L must be replaced with its alphabetical code: • L = 0 is S, • L = 1 is P, • L = 2 is D, • L = 3 is F, • L = 4 is G, • L = 5 is H ... • J is the vector sum of L and S: • J = (L+S), (L+S-1), (L+S-2), ...| L-S| Assign term symbols: The basic state of hydrogen atom is one electron in the lowest energy atom orbital: 1s. Therefore, the total orbital angle torque of all (one) electrons is L = l = 0, and the total electronspinnet is S = s = 1 /2. The use of the definition of the term symbol results in a 2S1/2 atomic term for the ground state of the H atom. This symbol is read: doublet Ace a half Exciting single hydrogen electrons to higher orbitals resulting in different nuclear states or conditions of the atom. Note that an H-atom with electron in a 3d and 10d orbital both results in 2D3/2 and 2D5/2 conditions, but on different energies. The lowest electron configuration of He is 1s2. The ground state of the neutral helium atom is therefore 1S0 since the total orbital and spinning momentum of this configuration is zero. In fact, any electron configuration (orbital population) consisting of a combination of closed shells or subshells will result in this (completely symmetrical 1S0-term. Therefore, in the designation of atomic terms, the contribution of closed subshell electrons can be neglected. What can't be neglected? The resulting angular moment of the open shell electrons in the atom! Because the angle momenta of each electron adds to the rest of the electrons weightorially, there will generally be more than one possible result of this supplement. It is our job to account for every possible way that the properties of the electrons will summarize and sort these possibilities into those corresponding to different conditions (total energies; nuclear states). We will seek to categorize each way the electrons add up by a complete description of l, ml, ms (is the same for all e's) of each electron: This is called a microstate. A given microstate is not necessarily a good description of the condition of the entire atom; sometimes many microstates are required to describe a given Term.To determine the states (terms) of a given Atom or Ion: • Write down the electronic configuration (ignore closed electrons) • Determine the number of different microstates that may represent this configuration. If you have e electrons in a single open subshell of 2l +1 orbitals, this value is #microstates (single open subshell) = (2 (2l + 1)) ! (2(2l +1)-e)! • Tabulate the number of microstates that have a given ML and MS • Decompose the table to conditions of elimination • Test the total degeneracy of the resulting conditions to take into account all the micro states counted in sections 2 and 3 • Determine the lowest term for the configuration of the Dog Rules. Summary Examples H (1s1) basic state term symbol is 2S1/2 He (1s2) Ground state term symbol is 1S0Han (1s12s1) A tense state configuration condition: 1S0, 3S1 { It is neither a 3S0 or a 3S-1 Term }B (1s22s22p1) {ground state} Term symbol: 2P1/2, 2P3/2 Spin orbit splitting is common so2P1/2is ground state. C (1s22s22p2) {lowest electron configuration} Calculate the number of possible electron ups in the specified configuration: There are 6!/4!2! = 15 microstates expected Write down all these possibilities:Tabulate total number of ML and MS Decompose this table to terms Check with reality: N (1s2 2s2 2p3) {lowest energy configuration) This configuration has 6!/3!3! = 20 microstates Draw all possibilities Tabulate totals Assign terms Assign TermsCheck with realityWhat are the nuclear state's term symbols as a result of the lowest energy configuration of O (1s2 2s2 2p4) ? Aha! We do not need to do this because the terms arising from p2 and p4 are exactly the same! Note, but ordering J levels is now invertedReality:If you think you have mastered the process of determining the states arising from a given electronic configuration, you should try Ti (1s22s22p63s23p64s23d2)Here is the answer depicted graphicsome results of this procedure for the game: Atomic term symbol Upcoming SlideShare Loading in ... 5 × 1 Like this presentation? Why not share! 1. . 2. F0r d1 system Total no. microstates = 10!/1!9! = 10 This means that the single electron can be arranged in this five sub orbitals in different 10 ways and representation will have different combination ML & MS value. +2 +1 0 -1 -2 ml = +2, +1, 0,-1 ,-2[for 1 e-] S = + 1/2 Hence 2S+1= 2 L = 2 in; e X = D 2D J =| L+S|,....| L-S| J=L-S {if orbital is less than half filled} J=L+S {if orbitals are more than half-filled} 3. • Determination of total wave function is micro states table for d2 confrigation. • example of free metallion (V3+) • Total no microstates = 45 • First we determine ML VALUE • ML = Ŵmli = ml1 + ml2 ml1 = +2, +1, 0 ,-1, -2 ml2 = +2 , +1, 0 -1, -2 +4....................-4 Middle values also possible +2 +1 0 -1 -2 4. • The range of total orbital quantum no. =+4, +3,+2,+1, 0 ,-1, -2,-3,-4 Next we determine total MS value MS =̄msi =ms1 +ms2 ms1 = +1/2 ,-1/2 ms2 = +1/2 ,-1/2 Total possible = +1 , 0 ,-1 By using these total spin quantum no. we can construct the micro states table. 5. ML/MS +1 0 -1 4 (2+,2-) 3 (2+,1+) (2+,1-) (2-,1+) (2-,1-) 2 (2+,0+) (2+,0-) (1+,1-)(2-,0+)(1-,1+) (2-,0-) 1 (1+,0+) (2+,-1+) (2+-1-) (1+,0-) (1-,0+)(2-,-1+) (1-,0-) (2-,-1-) 0 (1+,-1+) (2+,-2+) (2+,-2-) (1+,-1-)(0+,0-)(1+,1-)(2+,-2-) (1-,-1-)(2-,-2-) -1 (-1+,0+)(-2+,1+) (-2+,1-) (-1+,0-)(-1-,0+) (-2-,1+) (-1-,0-) (-2-,1-) -2 (-2+,0+) (-2+,0-) (-1+,-1-)(-2-,0+) (-2-,0-) -3 (-2+,-1+) (-2+,-1-) (-2-,-1+) (-2-,-1-) -4 (-2+,-2-) Construction table of Pauli's allowed microstates (a+, a+) and (a-,a-) are disallowed according to Pauli's exclusion principle 6. ML =±4 {1 ganger} ML =±3 {4 ganger} ML =±2 {5 ganger} ML =±1 {8 ganger} ML = 0 {9 ganger} OG MS= ±1 {10 ganger} MS = 0 {25 ganger} 7. a) første mulighet L = 4 & S = 0 ml Term will be 1G Total orbital degeneracy (2L + 1) (2S + 1) 2×4 + 1 = 9 J =| L+S|...| L-S| J =|4+0|...| 4-0| = 4 So there is no splitting of 1G Thus complete term symbol = 1G4 b) L = 3 & S = 1 Term will be 3F +2 +1 0 -1 -2 8. • Degeneracy (2L+1)(2S+1) = (2×3+1)(3) =21 • J =|3+1| ...| 3-1| • F term further splitting into three energy levels has J value 4, 3, 2 complete you terms are: 3F4, 3F3, 3F2 c) L = 2 & S = 0 term will be 1 D J = | 2 + 0 |.....| 2-0|= 2 1D2 there is no splitting degeneracy = (2×2 + 1) (1) = 5 d) L = 1 & S = 1 term will be 3 P J = | 1 + 1 | . . | | 1-1| = 2, 1.0 3P2, 3P1, 3P0 degeneracy=(2×1+1)(3) =9 9. • e) L = 0 & S = 0 visibility will be 1S j = 0 complete term symbol 1S0 degeneracy only one concepts derived for an electronic configuration have different energies. for example d2 configuation give rise five terms that are , 1G , 3F, 1D , 3P, 1S these five terms have different energies. These terms represent different inter electronic repulsion .the ground state term (lowest energy) can be determined using Hund's rule: 10. • 1) for a given collation ;the basic state (the term that has the lowest energy) is the one that has the highest spin multiplicity. Ground condition; therefore have the highest number of unpaired electrons and they provide maximum repulsion and high exchange energy. for example, ground state term for d2 conf. is 3F or 3P. • 2) if the two states have the same diversity the state will be highest value of L will be ground state. for d2; 3F & 3P both the same diversity, but3F higher value of L .3F has lower energy. Hence 3F is ground state • 3) for a given electronic configuation , if the diversity is the same and vales of L same for the nuclear states, then the state has lower j value will be lowest energy if subshells are less than half filled , the state has the highest value of j will be lower energy if the subshell is more than half filled. 11. Splitting of d2 configuration Prakash Bishnoi 6 months ago