jj COUPLING TREATMENT TO THE NONEQUIVALENT $f^nf^{n'}$ ELECTRONS FOR jj TERMS AND J LEVELS DETERMINATION

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Abstract: *Various coupling schemes are applied to smaller to heavy atoms to describe atomic structure and investigate atomic spectra. jj-coupling is important for heavy atoms in which spin-orbit interactions are dominant over the electrostatic interactions. Here jj-terms and J levels are determined for the nonequivalent $f^nf^{n'}$ (n & n' = 1-2) electrons from the analysis of all possible microstates. The determined jj terms are designated of the form $\left[\left(j_1 j_2 j_3 \ldots j_N\right)_J\right]$ notation.*

Keywords: *nonequivalent electron, $f^nf^{n'}$ configuration, jj terms, jj-coupling*
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Introduction

To obtain the energy levels from multielectron atomic systems, various types of interactions such as electron- electron interaction, spin-orbit interaction etc. are taken into consideration in the Hamiltonian. To describe these energy levels, they are designated by labels which called term symbols. The derivation of the electronic states arising from any given electronic configuration with equivalent or nonequivalent electron is by now a conventional topic in a chemistry course [1-2].

To determine the energy levels two coupling schemes LS-coupling and jj-coupling are the most widely used in atomic theory and spectroscopy. However, they are not suitable for investigation of some elements, so some other coupling schemes also used which are *LK* and *JK*-coupling schemes. The total number of levels with given J is the same for all coupling schemes. LS and jj-couplings are homogenous couplings since two electrons are coupled in pairs completely in a symmetric mode, whereas *LK* and *JK*-coupling are inhomogeneous, they are characterized by successive coupling of the momenta [3].

The LS coupling is most likely realized in smaller atoms, whereas the jj-coupling in the case of a heavy system or in atoms which are multiply ionized in which the effect of the spin-orbit coupling is no more negligible in relation to electrostatic effects [4-7].

The jj-coupling assumes that the orbital angular momenta, *l* of each electron is coupled to its spin-momneta, *s* to give its own angular momenta, *j* and all *j* coupled to give total angular momentum J, *j* values define a term and J values to the levels [8-9]. Symbolically the jj-coupling scheme is written as given by equation (1).

$$\{(\vec{l}_1\vec{s}_1)(\vec{l}_2\,\vec{s}_2)\} = (\vec{j}_1\,\vec{j}_2) = \vec{J} \qquad (1)$$

For an equivalent electronic system, the electron-electron interaction is almost larger than the spin-orbit interaction. Thus, for the nonequivalent electronic system the jj-coupling is of the greatest interest [10].

Here the possible jj terms arising from the nonequivalent electrons of $f^nf^{n'}$ (*n* & *n'* = 1-2) configurations occupying to the nonequivalent subshells are obtained from the analysis of all possible microstates and J levels to each jj term are determined.

Methodology

Different method have been developed for determination of the jj terms and J levels, for the equivalent electrons [8, 11-18] and nonequivalent electrons [8, 11, 13, 14, 18-21]. To derive the jj terms and J levels for the nonequivalent $f^nf^{n'}$ electrons, first of all, the total number of microstates for nonequivalent $f^n f^{n'}$ electrons are calculated by possible permutations. The calculated total microstates for nonequivalent $f^1\,f^1$, $f^1\,f^2$ & $f^2\,f^1$ and $f^2\,f^2$ electrons are 196, 1274 and 8281. After this the possible jj terms are determined by using equation (2) [13].

$$[(n+1)\times(n'+1)] \qquad (2)$$

where n and n' are represent the total number of electrons in subshells.

The determined possible jj terms are designated as $\left[(j_1, j_2, j_3, \ldots . j_N)_J\right]$ notation [8, 9], where the j_1, j_2, j_3, j_N are the total angular momenta of electrons. The possible number of jj terms for the nonequivalent $f^1\,f^1$, $f^1\,f^2$ & $f^2\,f^1$ and $f^2\,f^2$ electrons are 4, 6 and 9. The j values for f-orbital are 7/2 and 5/2, therefore these jj terms in $\left[(j_1, j_2, j_3, \ldots . j_N)_J\right]$ notation are given in Table 1.

Table 1. jj terms for $f^n f^{n'}$ configurations

$f^n f^{n'}$ configurations	jj terms
$f^1 f^1$ configuration	$\left(\frac{7}{2},\frac{7}{2}\right)\left(\frac{7}{2},\frac{5}{2}\right)\left(\frac{5}{2},\frac{7}{2}\right)\left(\frac{5}{2},\frac{5}{2}\right)$
$f^1 f^2$ configuration	$\left(\frac{7}{2},\frac{7}{2},\frac{7}{2}\right)\left(\frac{7}{2},\frac{7}{2},\frac{5}{2}\right)\left(\frac{7}{2},\frac{5}{2},\frac{5}{2}\right)\left(\frac{5}{2},\frac{7}{2},\frac{7}{2}\right)\left(\frac{5}{2},\frac{7}{2},\frac{5}{2}\right)\left(\frac{5}{2},\frac{5}{2},\frac{5}{2}\right)$
$f^2 f^1$ configuration	$\left(\frac{7}{2},\frac{7}{2},\frac{7}{2}\right)\left(\frac{7}{2},\frac{7}{2},\frac{5}{2}\right)\left(\frac{7}{2},\frac{5}{2},\frac{7}{2}\right)\left(\frac{7}{2},\frac{5}{2},\frac{5}{2}\right)\left(\frac{5}{2},\frac{5}{2},\frac{7}{2}\right)\left(\frac{5}{2},\frac{5}{2},\frac{5}{2}\right)$
$f^2 f^2$ configuration	$\left(\frac{7}{2},\frac{7}{2},\frac{7}{2},\frac{7}{2}\right)\left(\frac{7}{2},\frac{7}{2},\frac{7}{2},\frac{5}{2}\right)\left(\frac{7}{2},\frac{7}{2},\frac{5}{2},\frac{5}{2}\right)\left(\frac{7}{2},\frac{5}{2},\frac{7}{2},\frac{7}{2}\right)\left(\frac{7}{2},\frac{5}{2},\frac{7}{2},\frac{5}{2}\right)\left(\frac{7}{2},\frac{5}{2},\frac{5}{2},\frac{5}{2}\right)\left(\frac{5}{2},\frac{5}{2},\frac{7}{2},\frac{7}{2}\right)\left(\frac{5}{2},\frac{5}{2},\frac{7}{2},\frac{5}{2}\right)\left(\frac{5}{2},\frac{5}{2},\frac{5}{2},\frac{5}{2}\right)$

Further, total number of microstates associated with a particular jj term counted by using equation (3) [13].

$$\left[\frac{(2\ell)!(2\ell+2)!}{i!(2\ell-i)!(n-i)!(2\ell+2+i-n)!}\right] x \left[\frac{(2\ell')!(2\ell'+2)!}{i!(2\ell'-i)!(n'-i)!(2\ell'+2+i-n')!}\right] \qquad (3)$$

where n and n' represent the number of electrons in partially filled subshells, ℓ and ℓ' represent values of orbital angular quantum numbers and the value of i is constrained such that, $[n \geq i \geq 0]$ for subshell less than half full, $[2\ell \geq i \geq 0]$ for subshell half full and $[2\ell \geq i \geq n-2\ell-2]$ for subshell more than half. The microstates for each jj terms for the nonequivalent $f^1\,f^1$, $f^1\,f^2$ & $f^1\,f^2$ and $f^2\,f^2$ electrons are represented in Table 2.

Table 2. Microstates for each jj term for $f^n f^{n'}$ configuration

$f^n f^{n'}$ configurations jj terms with microstates						
$f^1 f^1$ configuration		jj terms				
$\left(\frac{7}{2},\frac{7}{2}\right)$	$\left(\frac{7}{2},\frac{5}{2}\right)$	$\left(\frac{5}{2},\frac{7}{2}\right)$	$\left(\frac{5}{2},\frac{5}{2}\right)$			196
64	48	48	36			
$f^1 f^2$ configuration		jj terms				
$\left(\frac{7}{2},\frac{7}{2},\frac{7}{2}\right)$	$\left(\frac{7}{2},\frac{7}{2},\frac{5}{2}\right)$	$\left(\frac{7}{2},\frac{5}{2},\frac{5}{2}\right)$	$\left(\frac{5}{2},\frac{7}{2},\frac{7}{2}\right)$	$\left(\frac{5}{2},\frac{7}{2},\frac{5}{2}\right)$	$\left(\frac{5}{2},\frac{5}{2},\frac{5}{2}\right)$	1274
224	384	120	168	288	90	
$f^2 f^1$ configuration		jj terms				

$\left(\frac{7}{2},\frac{7}{2},\frac{7}{2}\right)$	$\left(\frac{7}{2},\frac{7}{2},\frac{5}{2}\right)$	$\left(\frac{7}{2},\frac{5}{2},\frac{7}{2}\right)$	$\left(\frac{7}{2},\frac{5}{2},\frac{5}{2}\right)$	$\left(\frac{5}{2},\frac{5}{2},\frac{7}{2}\right)$	$\left(\frac{5}{2},\frac{5}{2},\frac{5}{2}\right)$	1274
224	168	384	288	120	90	
f^2f^2 configuration		jj terms				
$\left(\frac{7}{2},\frac{7}{2},\frac{7}{2},\frac{7}{2}\right)$	$\left(\frac{7}{2},\frac{7}{2},\frac{7}{2},\frac{5}{2}\right)$ & $\left(\frac{7}{2},\frac{7}{2},\frac{5}{2},\frac{7}{2}\right)$	$\left(\frac{5}{2},\frac{5}{2},\frac{7}{2},\frac{7}{2}\right)$ & $\left(\frac{7}{2},\frac{7}{2},\frac{5}{2},\frac{5}{2}\right)$	$\left(\frac{7}{2},\frac{5}{2},\frac{7}{2},\frac{5}{2}\right)$	$\left(\frac{7}{2},\frac{5}{2},\frac{5}{2},\frac{5}{2}\right)$ & $\left(\frac{5}{2},\frac{5}{2},\frac{7}{2},\frac{5}{2}\right)$	$\left(\frac{5}{2},\frac{5}{2},\frac{5}{2},\frac{5}{2}\right)$	8281
784	1334	420	2304	720	225	

Once the jj terms and total microstates associated with jj terms have been determined, a microstate table for each jj term is constructed and M_J values for each microstate is determines and all microstates for given jj term are arranged in another microstate table with M_J (J, J-1, …….., -J) from which J levels for each jj term are determined by elimination of microstates associated with particular M_J starting from maximum M_J and finally move to lowest possible M_J. The microstate table (Table 3) all jj terms to the nonequivalent f^1f^1 electrons is constructed by arranging two electrons with different j values is and M_J values for all microstates are calculated and same is done for other nonequivalent $f^nf^{n'}$ electrons.

Table 3. Microstates for different jj terms of f^1 f^1 configuration

jj term $(7/2, 7/2)$														
j_1	j_2	M_J	j_1	j_2	M_J	j_1	j_2	M_J	j_1	j_2	M_J	j_1	j_2	M_J
7/2	7/2	**7**	5/2	7/2	**6**	3/2	7/2	**5**	1/2	7/2	**4**	-1/2	7/2	**3**
7/2	5/2	**6**	5/2	5/2	**5**	3/2	5/2	**4**	1/2	5/2	**3**	-1/2	5/2	**2**
7/2	3/2	**5**	5/2	3/2	**4**	3/2	3/2	**3**	1/2	3/2	**2**	-1/2	3/2	**1**
7/2	1/2	**4**	5/2	1/2	**3**	3/2	1/2	**2**	1/2	1/2	**1**	-1/2	1/2	**0**
7/2	-1/2	**3**	5/2	-1/2	**2**	3/2	-1/2	**1**	1/2	-1/2	**0**	-1/2	-1/2	**-1**
7/2	-3/2	**2**	5/2	-3/2	**1**	3/2	-3/2	**0**	1/2	-3/2	**-1**	-1/2	-3/2	**-2**
7/2	-5/2	**1**	5/2	-5/2	**0**	3/2	-5/2	**-1**	1/2	-5/2	**-2**	-1/2	-5/2	**-3**
7/2	-7/2	**0**	5/2	-7/2	**-1**	3/2	-7/2	**-2**	1/2	-7/2	**-3**	-1/2	-7/2	**-4**
-3/2	7/2	**2**	-3/2	-1/2	**-2**	-5/2	7/2	**1**	-5/2	-1/2	**-3**	-7/2	7/2	**0**
-3/2	5/2	**1**	-3/2	-3/2	**-3**	-5/2	5/2	**0**	-5/2	-3/2	**-4**	-7/2	5/2	**-1**
-3/2	3/2	**0**	-3/2	-5/2	**-4**	-5/2	3/2	**-1**	-5/2	-5/2	**-5**	-7/2	3/2	**-2**
-3/2	1/2	**-1**	-3/2	-7/2	**-5**	-5/2	1/2	**-2**	-5/2	-7/2	**-6**	-7/2	1/2	**-3**
-7/2	-1/2	**-4**	-7/2	-3/2	**-5**	-7/2	-5/2	**-6**	-7/2	-7/2	**-7**			
jj term $(7/2, 5/2)$														
j_1	j_2	M_J	j_1	j_2	M_J	j_1	j_2	M_J	j_1	j_2	M_J	j_1	j_2	M_J
7/2	5/2	**6**	5/2	5/2	**5**	3/2	5/2	**4**	1/2	5/2	**3**	-1/2	5/2	**2**
7/2	3/2	**5**	5/2	3/2	**4**	3/2	3/2	**3**	1/2	3/2	**2**	-1/2	3/2	**1**
7/2	1/2	**4**	5/2	1/2	**3**	3/2	1/2	**2**	1/2	1/2	**1**	-1/2	1/2	**0**
7/2	-1/2	**3**	5/2	-1/2	**2**	3/2	-1/2	**1**	1/2	-1/2	**0**	-1/2	-1/2	**-1**
7/2	-3/2	**2**	5/2	-3/2	**1**	3/2	-3/2	**0**	1/2	-3/2	**-1**	-1/2	-3/2	**-2**
7/2	-5/2	**1**	5/2	-5/2	**0**	3/2	-5/2	**-1**	1/2	-5/2	**-2**	-1/2	-5/2	**-3**
-3/2	5/2	**1**	-3/2	-3/2	**-3**	-5/2	1/2	**-2**	-7/2	5/2	**-1**	-7/2	-3/2	**-5**
-3/2	3/2	**0**	-3/2	-5/2	**-4**	-5/2	-1/2	**-3**	-7/2	3/2	**-2**	-7/2	-5/2	**-6**
-3/2	1/2	**-1**	-5/2	5/2	**0**	-5/2	-3/2	**-4**	-7/2	1/2	**-3**			
-3/2	-1/2	**-2**	-5/2	3/2	**-1**	-5/2	-5/2	**-5**	-7/2	-1/2	**-4**			
jj term $(5/2, 7/2)$														

j_1	j_2	M_J	j_1	j_2	M_J	j_1	j_2	M_J	j_1	j_2	M_J	j_1	j_2	M_J
5/2	7/2	**6**	3/2	7/2	**5**	1/2	7/2	**4**	-1/2	7/2	**3**	-3/2	7/2	**2**
5/2	5/2	**5**	3/2	5/2	**4**	1/2	5/2	**3**	-1/2	5/2	**2**	-3/2	5/2	**1**
5/2	3/2	**4**	3/2	3/2	**3**	1/2	3/2	**2**	-1/2	3/2	**1**	-3/2	3/2	**0**
5/2	1/2	**3**	3/2	1/2	**2**	1/2	1/2	**1**	-1/2	1/2	**0**	-3/2	1/2	**-1**
5/2	-1/2	**2**	3/2	-1/2	**1**	1/2	-1/2	**0**	-1/2	-1/2	**-1**	-3/2	-1/2	**-2**
5/2	-3/2	**1**	3/2	-3/2	**0**	1/2	-3/2	**-1**	-1/2	-3/2	**-2**	-3/2	-3/2	**-3**
5/2	-5/2	**0**	3/2	-5/2	**-1**	1/2	-5/2	**-2**	-1/2	-5/2	**-3**	-3/2	-5/2	**-4**
5/2	-7/2	**-1**	3/2	-7/2	**-2**	1/2	-7/2	**-3**	-1/2	-7/2	**-4**	-3/2	-7/2	**-5**
-5/2	7/2	**1**	-5/2	3/2	**-1**	-5/2	-1/2	**-3**	-5/2	-5/2	**-5**			
-5/2	5/2	**0**	-5/2	1/2	**-2**	-5/2	-3/2	**-4**	-5/2	-7/2	**-6**			
jj term $(5/2, 5/2)$														
j_1	j_2	M_J	j_1	j_2	M_J	j_1	j_2	M_J	j_1	j_2	M_J	j_1	j_2	M_J
5/2	5/2	**5**	3/2	5/2	**4**	1/2	5/2	**3**	-1/2	5/2	**2**	-3/2	5/2	**1**
5/2	3/2	**4**	3/2	3/2	**3**	1/2	3/2	**2**	-1/2	3/2	**1**	-3/2	3/2	**0**
5/2	1/2	**3**	3/2	1/2	**2**	1/2	1/2	**1**	-1/2	1/2	**0**	-3/2	1/2	**-1**
5/2	-1/2	**2**	3/2	-1/2	**1**	1/2	-1/2	**0**	-1/2	-1/2	**-1**	-3/2	-1/2	**-2**
5/2	-3/2	**1**	3/2	-3/2	**0**	1/2	-3/2	**-1**	-1/2	-3/2	**-2**	-3/2	-3/2	**-3**
5/2	-5/2	**0**	3/2	-5/2	**-1**	1/2	-5/2	**-2**	-1/2	-5/2	**-3**	-3/2	-5/2	**-4**
-5/2	5/2	**0**	-5/2	1/2	**-2**	-5/2	-3/2	**-4**						
-5/2	3/2	**-1**	-5/2	-1/2	**-3**	-5/2	-5/2	**-5**						

Determination of J levels for jj terms

J level for jj term are obtained by elimination of microstates from microstates associated with a particular J level starting from the maximum M_J value and followed for next J levels and finally move to lowest possible M_J value.

J levels determination and microstates elimination for nonequivalent f^1f^1 electrons

For $\left(\frac{7}{2},\frac{7}{2}\right)$ jj term of the nonequivalent f^1f^1 electrons, 15 microstates (M_J =7 to M_J = -7) associated with maximum M_J=7 are eliminated from Table 4 which result into J=7 level and the next maximum M_J =6, which yield another J=6 level by elimination of 13 microstates (M_J =6 to M_J = -6), and follow the same procedure the continuous elimination of 11, 9,7, 5, 3 and 1 microstates associated with M_J = 5, 4, 3, 2, 1 and 0, result into J=5, 4, 3, 2, 1 and 0 levels for this term. Using the same procedure for other jj terms for the nonequivalent f^1f^1 electrons and for the nonequivalent $f^1 f^2$, $f^2 f^1$ and $f^2 f^2$ electrons the J levels are determined. J levels determination for all jj terms for the nonequivalent f^1 f^1 electrons are represented in Table 4 to Table 6.

Table 4. J levels for $(7/2, 7/2)$ jj term for $f^1 f^1$ configuration

M_J	Microstates	Microstates left after the sequential elimination of J levels							
7	1	0							
6	2	1	0						
5	3	2	1	0					
4	4	3	2	1	0				
3	5	4	3	2	1	0			
2	6	5	4	3	2	1	0		
1	7	6	5	4	3	2	1	0	
0	8	7	6	5	4	3	2	1	0
-1	7	6	5	4	3	2	1	0	
-2	6	5	4	3	2	1	0		
-3	5	4	3	2	1	0			
-4	4	3	2	1	0				

-5	3	2	1	0					
-6	2	1	0						
-7	1	0							
Microstates	64	49	36	25	16	9	4	1	0
J levels	7	6	5	4	3	2	1	0	

Table 5. J levels for $(7/2,5/2)$ and $(5/2,7/2)$ jj terms for $f^1 f^1$ configuration

M_J	Microstates	Microstates left after the sequential elimination of J levels					
6	1	0					
5	2	1	0				
4	3	2	1	0			
3	4	3	2	1	0		
2	5	4	3	2	1	0	
1	6	5	4	3	2	1	0
0	6	5	4	3	2	1	0
-1	6	5	4	3	2	1	0
-2	5	4	3	2	1	0	
-3	4	3	2	1	0		
-4	3	2	1	0			
-5	2	1	0				
-6	1	0					
Microstates	48	35	24	15	8	3	0
J levels	6	5	4	3	2	1	

Table 6. J levels for $(5/2,5/2)$ jj term for $f^1 f^1$ configuration

M_J	Microstates	Microstates left after the sequential elimination of J levels					
5	1	0					
4	2	1	0				
3	3	2	1	0			
2	4	3	2	1	0		
1	5	4	3	2	1	0	
0	6	5	4	3	2	1	0
-1	5	4	3	2	1	0	
-2	4	3	2	1	0		
-3	3	2	1	0			
-4	2	1	0				
-5	1	0					
Microstates	36	25	16	9	4	1	0
J levels	5	4	3	2	1	0	

J levels determination and microstates elimination for nonequivalent f^1f^2 and f^2f^1 electrons

J levels determination for all jj terms for the nonequivalent f^1f^2 and f^2 f^1 electrons are represented in Table 7 to Table 12.

Table 7. J levels for $(7/2, 7/2, 7/2)$ jj term for $f^1 f^2$ and $f^2 f^1$ configurations

M_J	Micro states	Microstates left after the sequential removal of different J levels									
19/2	1	0									
17/2	2	1	0								
15/2	4	3	2	0							
13/2	6	5	4	2	0						
11/2	9	8	7	5	3	0					
9/2	12	11	10	8	6	3	0				
7/2	16	15	14	12	10	7	4	0			
5/2	19	18	17	15	13	10	7	3	0		
3/2	21	20	19	17	15	12	9	5	2	0	
1/2	22	21	20	18	16	13	10	6	3	1	0
-1/2	22	21	20	18	16	13	10	6	3	1	0
-3/2	21	20	19	17	15	12	9	5	2	0	
-5/2	19	18	17	15	13	-10	7	3	0		
-7/2	16	15	14	12	10	7	4	0			
-9/2	12	11	10	8	6	3	0				
-11/2	9	8	7	5	3	0					
-13/2	6	5	4	2	0						
-15/2	4	3	2	0							
-17/2	2	1	0								
-19/2	1	0									
Micro states	224	204	186	154	126	90	60	28	10	2	0
J levels	19/2	17/2	15/2 (2)	13/2 (2)	11/2 (3)	9/2 (3)	7/2 (4)	5/2 (3)	3/2 (2)	1/2	

Table 8. J levels for $(5/2, 5/2, 5/2)$ jj term for $f^1 f^2$ and $f^2 f^1$ configurations

M_J	Microstates	Microstates left after the sequential removal of different J levels						
13/2	1	0						
11/2	2	1	0					
9/2	4	3	2	0				
7/2	6	5	4	2	0			
5/2	9	8	7	5	3	0		
3/2	11	10	9	7	5	2	0	
1/2	12	11	10	8	6	3	1	0
-1/2	12	11	10	8	6	3	1	0
-3/2	11	10	9	7	5	2	0	
-5/2	9	8	7	5	3	0		
-7/2	6	5	4	2	0			
-9/2	4	3	2	0				
-11/2	2	1	0					

-13/2	1	0						
Microstates	90	76	64	44	28	10	2	0
J levels	13/2	11/2	9/2(2)	7/2(2)	5/2(3)	3/2(2)	1/2	

Table 9. J levels for $(7/2, 7/2, 5/2)$ jj term for $f^1 f^2$ configuration and $(7/2, 5/2, 7/2)$ jj term for $f^2 f^1$ configurations

M_J	Microstates	Microstates left after the sequential removal of different J levels									
19/2	1	0									
17/2	3	2	0								
15/2	6	4	2	0							
13/2	10	8	6	4	0						
11/2	15	13	11	9	5	0					
9/2	21	19	17	15	11	6	0				
7/2	27	25	23	21	17	12	6	0			
5/2	33	31	29	27	23	18	12	6	0		
3/2	37	35	33	31	27	22	16	10	4	0	
1/2	39	37	35	33	29	24	20	14	8	4	0
-1/2	39	37	35	33	29	24	20	14	8	4	0
-3/2	37	35	33	31	27	22	16	10	4	0	
-5/2	33	31	29	27	23	18	12	6	0		
-7/2	27	25	23	21	17	12	6	0			
-9/2	21	19	17	15	11	6	0				
-11/2	15	13	11	9	5	0					
-13/2	10	8	6	4	0						
-15/2	6	4	2	0							
-17/2	3	2	0								
-19/2	1	0									
Microstates	384	364	312	280	224	152	108	60	24	8	0
J levels	19/2	17/2 (2)	15/2 (2)	13/2 (4)	11/2 (5)	9/2 (6)	7/2 (6)	5/2 (6)	3/2 (4)	1/2 (4)	

Table 10. J levels for $(7/2, 5/2, 5/2)$ jj term for $f^1 f^2$ configuration and $(5/2, 5/2, 7/2)$ jj term for $f^2 f^1$ configuration

M_J	Microstates	Microstates left after the sequential removal of different J levels							
15/2	1	0							
13/2	2	1	0						
11/2	4	3	2	0					
9/2	6	5	4	2	0				
7/2	9	8	7	5	3	0			
5/2	11	10	9	7	5	2	0		
3/2	13	12	11	9	7	4	2	0	
1/2	14	13	12	10	8	5	3	1	0

-1/2	14	13	12	10	8	5	3	1	0
-3/2	13	12	11	9	7	4	2	0	
-5/2	11	10	9	7	5	2	0		
-7/2	9	8	7	5	3	0			
-9/2	6	5	4	2	0				
-11/2	4	3	2	0					
-13/2	2	1	0						
-15/2	1	0							
Microstates	120	104	90	66	46	22	10	2	0
J levels	15/2	13/2	11/2(2)	9/2(2)	7/2(3)	5/2(2)	3/2(2)	1/2	

Table 11. J levels for $(5/2, 7/2, 7/2)$ jj term for $f^1 f^2$ configuration and $(7/2, 7/2, 5/2)$ jj term for $f^2 f^1$ configuration

M_J	Microstates	Microstates left after the sequential removal of different J levels								
17/2	1	0								
15/2	2	1	0							
13/2	4	3	2	0						
11/2	6	5	4	2	0					
9/2	9	8	7	5	3	0				
7/2	12	11	10	8	6	3	0			
5/2	15	14	13	11	9	6	3	0		
3/2	17	16	15	13	11	8	5	2	0	
1/2	18	17	16	14	12	9	6	3	1	0
-1/2	18	17	16	14	12	9	6	3	1	0
-3/2	17	16	15	13	11	8	5	2	0	
-5/2	15	14	13	11	9	6	3	0		
-7/2	12	11	10	8	6	3	0			
-9/2	9	8	7	5	3	0				
-11/2	6	5	4	2	0					
-13/2	4	3	2	0						
-15/2	2	1	0							
-17/2	1	0								
Microstates	168	150	134	106	81	52	28	10	2	0
J levels	17/2	15/2	13/2(2)	11/2(2)	9/2(3)	7/2(3)	5/2(3)	3/2(2)	1/2	

Table 12. J levels for $(5/2, 7/2, 5/2)$ jj term for $f^1 f^2$ configuration and $(7/2, 5/2, 5/2)$ jj term for $f^2 f^1$ configuration

M_J	Microstates	Microstates left after sequential removal of different J levels								
17/2	1	0								
15/2	3	2	0							
13/2	6	5	3	0						
11/2	10	9	7	4	0					
9/2	16	15	13	10	6	0				
7/2	21	20	18	15	11	5	0			
5/2	26	25	23	20	16	10	5	0		

3/2	29	28	26	23	19	13	8	3	0	
1/2	32	31	29	26	22	16	11	6	3	0
-1/2	32	31	29	26	22	16	11	6	3	0
-3/2	29	28	26	23	19	13	8	3	0	
-5/2	26	25	23	20	16	10	5	0		
-7/2	21	20	18	15	11	5	0			
-9/2	16	15	13	10	6	0				
-11/2	10	9	7	4	0					
-13/2	6	5	3	0						
-15/2	3	2	0							
-17/2	1	0								
Microstates	288	270	238	196	148	88	48	18	6	0
J levels	17/2	15/2(2)	13/2(3)	11/2(4)	9/2(6)	7/2(5)	5/2(5)	3/2(3)	1/2(3)	

J levels determination and microstates elimination for the nonequivalent f^2f^2 electrons

J levels determination for all jj terms for the nonequivalent f^2 f^2 electrons are represented in Table 13 to Table 18.

Table 13. J levels for $(7/2,\ 7/2,\ 7/2\ ,7/2,)$ jj term for f^2 f^2 configuration

M_J	Micro states	Microstates left after the sequential removal of different J levels												
12	1	0												
11	2	1	0											
10	5	4	3	0										
9	8	7	6	3	0									
8	14	13	12	9	6	0								
7	20	19	18	15	12	6	0							
6	30	29	28	25	22	16	10	0						
5	38	37	36	33	30	24	18	8	0					
4	49	48	47	44	41	35	29	19	11	0				
3	56	55	54	51	48	42	36	26	18	7	0			
2	65	64	63	60	57	51	45	35	27	16	9	0		
1	68	67	66	63	60	54	48	38	30	19	12	3	0	
0	72	71	70	67	64	58	52	42	34	23	16	7	4	0
-1	68	67	66	63	60	54	48	38	30	19	12	3	0	
-2	65	64	63	60	57	51	45	35	27	16	9	0		
-3	56	55	54	51	48	42	36	26	18	7	0			
-4	49	48	47	44	41	35	29	19	11	0				
-5	38	37	36	33	30	24	18	8	0					
6	30	29	28	25	22	16	10	0						
-7	20	19	18	15	12	6	0							
-8	14	13	12	9	6	0								
-9	8	7	6	3	0									
-10	5	4	3	0										
-11	2	1	0											
-12	1	0												
Micro states	784	759	736	673	616	514	424	294	206	107	58	13	4	0

J levels	12	11	10 (3)	9 (3)	8 (6)	7 (6)	6 (10)	5 (8)	4 (11)	3 (7)	2 (9)	1 (3)	0 (4)	

Table 14. J levels for $(7/2, 7/2, 7/2, 5/2,)$ and $(7/2, 5/2, 7/2, 7/2,)$ jj terms for $f^2 f^2$ configuration

M_J	Micro states	Microstates left after sequential removal of different J levels												
12	1	0												
11	3	2	0											
10	7	6	4	0										
9	13	12	10	6	0									
8	22	21	19	15	9	0								
7	34	33	31	27	21	12	0							
6	49	48	46	42	36	27	15	0						
5	66	65	63	59	53	44	32	17	0					
4	83	82	80	76	70	61	49	34	17	0				
3	99	98	96	92	86	77	65	50	33	16	0			
2	112	111	109	105	99	90	78	63	46	29	13	0		
1	121	120	118	114	108	99	87	72	55	38	22	9	0	
0	124	123	121	117	111	102	90	75	58	41	25	12	3	0
-1	121	120	118	114	108	99	87	72	55	38	22	9	0	
-2	112	111	109	105	99	90	78	63	46	29	13	0		
-3	99	98	96	92	86	77	65	50	33	16	0			
-4	83	82	80	76	70	61	49	34	17	0				
-5	66	65	63	59	53	44	32	17	0					
-6	49	48	46	42	36	27	15	0						
-7	34	33	31	27	21	12	0							
-8	22	21	19	15	9	0								
-9	13	12	10	6	0									
-10	7	6	4	0										
-11	3	2	0											
-12	1	0												
Micro states	1344	1319	1273	1189	1075	922	742	547	360	207	95	30	3	0
J levels	12	11 (2)	10 (4)	9 (6)	8 (9)	7 (12)	6 (15)	5 (17)	4 (17)	3 (16)	2 (13)	1 (9)	0 (3)	

Table 15. J levels for $(5/2, 5/2, 5/2, 5/2,)$ jj term for $f^2 f^2$ configuration

M_J	Microstates	Microstates left after the sequential removal of different J levels								
8	1	0								
7	2	1	0							
6	5	4	3	0						
5	8	7	6	3	0					
4	14	13	12	9	6	0				
3	18	17	16	13	10	4	0			
2	24	23	22	19	16	10	6	0		
1	26	25	24	21	18	12	8	2	0	
0	29	28	27	24	21	15	11	5	3	0
-1	26	25	24	21	18	12	8	2	0	
-2	24	23	22	19	16	10	6	0		

-3	18	17	16	13	10	4	0			
-4	14	13	12	9	6	0				
-5	8	7	6	3	0					
-6	5	4	3	0						
-7	2	1	0							
-8	1	0								
Microstates	225	208	193	154	121	67	39	9	3	0
J levels	8	7	6(3)	5(3)	4(6)	3(4)	2(6)	1(2)	0(3)	

Table 16. J levels for $(7/2,\ 7/2,\ 5/2\ ,5/2,)$ and $(5/2,\ 5/2,\ 7/2\ ,7/2,)$ jj terms for $f^2\ f^2$ configuration

M_J	Microstates	Microstates left after the sequential removal of different J levels										
10	1	0										
9	2	1	0									
8	5	4	3	0								
7	8	7	6	3	0							
6	14	13	12	9	6	0						
5	19	18	17	14	11	5	0					
4	27	26	25	22	19	13	8	0				
3	32	31	30	27	24	18	13	5	0			
2	39	38	37	34	31	25	20	12	7	0		
1	41	40	39	36	33	27	22	14	9	2	0	
0	44	43	42	39	36	30	25	17	12	5	3	0
-1	41	40	39	36	33	27	22	14	9	2	0	
-2	39	38	37	34	31	25	20	12	7	0		
-3	32	31	30	27	24	18	13	5	0			
-4	27	26	25	22	19	13	8	0				
-5	19	18	17	14	11	5	0					
-6	14	13	12	9	6	0						
-7	8	7	6	3	0							
-8	5	4	3	0								
-9	2	1	0									
-10	1	0										
Microstates	420	399	380	329	284	206	151	79	44	9	3	0
J levels	10	9	8(3)	7(3)	6(6)	5(5)	4(8)	3(5)	2(7)	1(2)	0(3)	

Table 17. J levels for $(7/2,\ 5/2,\ 5/2\ ,5/2,)$ and $(5/2,\ 5/2,\ 7/2\ ,5/2,)$ jj terms for $f^2\ f^2$ configuration

M_J	Microstates	Microstates left after the sequential removal of different J levels									
10	1	0									
9	3	2	0								
8	7	6	4	0							
7	13	12	10	6	0						
6	22	21	19	15	9	0					
5	33	32	30	26	20	11	0				
4	45	44	42	38	32	23	12	0			
3	57	56	54	50	44	35	24	12	0		
2	67	66	64	60	54	45	34	22	10	0	

1	74	73	71	67	61	52	41	29	17	7	0
0	76	75	73	69	63	54	43	31	19	9	2
-1	74	73	71	67	61	52	41	29	17	7	0
-2	67	66	64	60	54	45	34	22	10	0	
-3	57	56	54	50	44	35	24	12	0		
-4	45	44	42	38	32	23	12	0			
-5	33	32	30	26	20	11	0				
-6	22	21	19	15	9	0					
-7	13	12	10	6	0						
-8	7	6	4	0							
-9	3	2	0								
-10	1	0									
Microstates	720	699	661	593	503	386	265	157	73	23	2
J levels	10	9(2)	8(4)	7(6)	6(9)	5(11)	4(12)	3(12)	2(10)	1(7)	0(2)

Table 18. J levels for $(7/2, 5/2, 7/2, 5/2,)$ jj term for $f^2 f^2$ configuration

M_J	Micro states	Microstates left after the sequential removal of different J levels												
12	1	0												
11	4	3	0											
10	10	9	6	0										
9	20	19	16	10	0									
8	35	34	31	25	15	0								
7	56	55	52	46	36	21	0							
6	82	81	78	72	62	47	26	0						
5	112	111	108	102	92	77	56	30	0					
4	143	142	139	133	123	108	87	61	31	0				
3	172	171	168	162	152	137	116	90	60	29	0			
2	196	195	192	186	176	161	140	114	84	53	24	0		
1	212	211	208	202	192	177	156	130	100	69	40	16	0	
0	218	217	214	208	198	183	162	136	106	75	46	22	6	0
-1	212	211	208	202	192	177	156	130	100	69	40	16	0	
-2	196	195	192	186	176	161	140	114	84	53	24	0		
-3	172	171	168	162	152	137	116	90	60	29	0			
-4	143	142	139	133	123	108	87	61	31	0				
-5	112	111	108	102	92	77	56	30	0					
-6	82	81	78	72	62	47	26	0						
-7	56	55	52	46	36	21	0							
-8	35	34	31	25	15	0								
-9	20	19	16	10	0									
-10	10	9	6	0										
-11	4	3	0											
-12	1	0												
Micro states	2304	2279	2210	2084	1894	1639	1324	986	656	377	174	54	6	0
J levels	12	11 (3)	10 (6)	9 (10)	8 (15)	7 (21)	6 (26)	5 (30)	4 (31)	3 (29)	2 (24)	1 (6)	0 (6)	

Results and Discussion

J levels determined for all the jj terms for the nonequivalent $f^n f^{n'}$ electrons (n = 1-2, n' = 1-2) are represented in Table 19. The ground state jj terms determined for these electrons are $\left(\frac{5}{2},\frac{5}{2}\right)$ for f^1f^1, $\left(\frac{5}{2},\frac{5}{2},\frac{5}{2}\right)$ for $f^1 f^2$ and $f^2 f^1$ and $\left(\frac{5}{2},\frac{5}{2},\frac{5}{2},\frac{5}{2}\right)$ f^2f^2 electrons. The jj terms and J levels for f^1 f^1 electrons are shown in Figure 1.

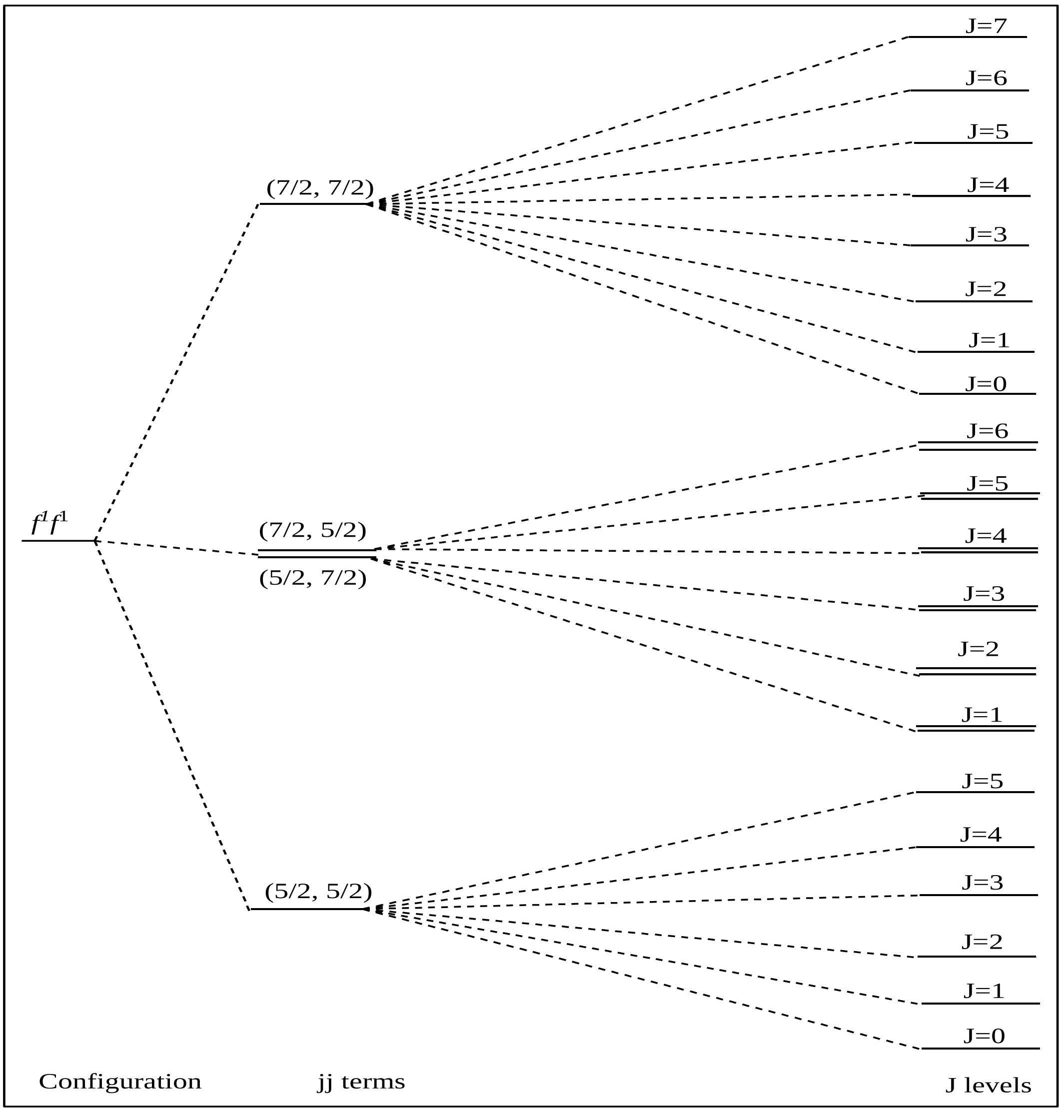

Figure 1. Schematic representation of jj terms and J levels for the nonequivalent $f^1 f^1$ electrons

Table 19. jj terms and J levels for different $f^n f^{n'}$ configurations

$f^1 f^1$ configuration
$\left[\left(\frac{7}{2},\frac{7}{2}\right) 7,6,5,4,3,2,1,0\right], \left[\left(\frac{7}{2},\frac{5}{2}\right) \& \left(\frac{5}{2},\frac{7}{2}\right) 6,5,4,3,2,1\right], \left[\left(\frac{5}{2},\frac{5}{2}\right) 5,4,3,2,1,0\right]$
$f^1 f^2$ configuration
$\left[\left(\frac{7}{2},\frac{7}{2},\frac{7}{2}\right) 19/2, 17/2, 15/2(2), 13/2(2), 11/2(3), 9/2(3), 7/2(4), 5/2(3), 3/2(2), 1/2\right]$
$\left[\left(\frac{7}{2},\frac{7}{2},\frac{5}{2}\right) 19/2, 17/2(2), 15/2(2), 13/2(4), 11/2(5), 9/2(6), 7/2(6), 5/2(6), 3/2(4), 1/2(4)\right]$

$\left[\left(\frac{7}{2},\frac{5}{2},\frac{5}{2}\right) 15/2, 13/2, 11/2(2), 9/2(2), 7/2(3), 5/2(2), 3/2(2), 1/2\right]$
$\left[\left(\frac{5}{2},\frac{7}{2},\frac{7}{2}\right) 17/2, 15/2, 13/2(2), 11/2(2), 9/2(3), 7/2(3), 5/2(3), 3/2(2), 1/2\right]$
$\left[\left(\frac{5}{2},\frac{7}{2},\frac{5}{2}\right) 17/2, 15/2(2), 13/2(3), 11/2(4), 9/2(6), 7/2(5), 5/2(5), 3/2(3), 1/2(3)\right]$
$\left[\left(\frac{5}{2},\frac{5}{2},\frac{5}{2}\right) 13/2, 11/2, 9/2(2), 7/2(2), 5/2(3), 3/2(2), 1/2\right]$
$f^2 f^1$ configuration
$\left[\left(\frac{7}{2},\frac{7}{2},\frac{7}{2}\right) 19/2, 17/2, 15/2(2), 13/2(2), 11/2(3), 9/2(3), 7/2(4), 5/2(3), 3/2(2), 1/2\right]$
$\left[\left(\frac{7}{2},\frac{5}{2},\frac{7}{2}\right) 19/2, 17/2(2), 15/2(2), 13/2(4), 11/2(5), 9/2(6), 7/2(6), 5/2(6), 3/2(4), 1/2(4)\right]$
$\left[\left(\frac{5}{2},\frac{5}{2},\frac{7}{2}\right) 15/2, 13/2, 11/2(2), 9/2(2), 7/2(3), 5/2(2), 3/2(2), 1/2\right]$
$\left[\left(\frac{7}{2},\frac{7}{2},\frac{5}{2}\right) 17/2, 15/2, 13/2(2), 11/2(2), 9/2(3), 7/2(3), 5/2(3), 3/2(2), 1/2\right]$
$\left[\left(\frac{7}{2},\frac{5}{2},\frac{5}{2}\right) 17/2, 15/2(2), 13/2(3), 11/2(4), 9/2(6), 7/2(5), 5/2(5), 3/2(3), 1/2(3)\right]$
$\left[\left(\frac{5}{2},\frac{5}{2},\frac{5}{2}\right) 13/2, 11/2, 9/2(2), 7/2(2), 5/2(3), 3/2(2), 1/2\right]$
$f^2 f^2$ configuration
$\left[\left(\frac{7}{2},\frac{7}{2},\frac{7}{2},\frac{7}{2}\right) 12,11,10(3),9(3),8(6),7(6),6(10),5(8),4(11),3(7),2(9),1(3),0(4)\right]$
$\left[\left\{\left(\frac{7}{2},\frac{7}{2},\frac{7}{2},\frac{5}{2}\right) \;\&\; \left(\frac{7}{2},\frac{7}{2},\frac{5}{2},\frac{7}{2}\right)\right\} 12,11(2), 10(4), 9(6), 8(9), 7(12), 6(15), 5(17),4(17),3(16),2(13),1(9),0(3)\right]$
$\left[\left\{\left(\frac{5}{2},\frac{5}{2},\frac{7}{2},\frac{7}{2}\right) \;\&\; \left(\frac{7}{2},\frac{7}{2},\frac{5}{2},\frac{5}{2}\right)\right\} 10,9, 8(3),7(3),6(6), 5(5),4(8),3(5),2(7),1(2),0(3)\right]$
$\left[\left(\frac{7}{2},\frac{5}{2},\frac{7}{2},\frac{5}{2}\right) 12,11(3),10(6),9(10),8(15),7(21),6(26),5(30),4(31),3(29),2(24),1(16),0(6)\right]$
$\left[\left\{\left(\frac{7}{2},\frac{5}{2},\frac{5}{2},\frac{5}{2}\right) \;\&\; \left(\frac{5}{2},\frac{5}{2},\frac{7}{2},\frac{5}{2}\right)\right\} 10,9(2),8(4),7(6),6(9),5(11),4(12),3(12),2(10),1(7),0(2)\right]$
$\left[\left(\frac{5}{2},\frac{5}{2},\frac{5}{2},\frac{5}{2}\right) 8,7,6(3), 5(3),4(6),3(4),2(6),1(2),0(3)\right]$

Conclusion

Using a simple method the jj terms and J levels are determined for the nonequivalent electrons for different $f^n f^{n'}$ configurations ($f^1 f^1$, $f^1 f^2$ & $f^2 f^1$ and $f^2 f^2$). These jj terms and J levels will be helpful in analysis of atomic structure and spectral properties of $f^n f^{n'}$ configurations and enrich knowledge about J levels and jj terms in theoretical inorganic chemistry.

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ОПРЕДЕЛЕНИЕ jj ТЕРМОВ И J УРОВНЕЙ НЕЭКВИВАЛЕНТНЫХ ЭЛЕКТРОНОВ

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jj-Термы и J уровни определены для неэквивалентных $f^nf^{n'}$ (n & n' = 1-2) электронов из анализа всех возможных микросостояний. Установленные jj термы обозначены в виде $\left[(j_1,j_2,j_3,\dots j_N)_J\right]$.

Ключевые слова: *неэквивалентные электроны, $f^nf^{n'}$конфигурации, jj-термы*

jj *TERMLƏRİNİN VƏ J SƏVİYYƏLƏRİNİN TƏYİN EDİLMƏSİ ÜÇÜN* QEYRİ *EKVİVALENT ELEKTRONLARA CÜTLƏŞMƏ İŞLƏNİLMƏSİNİN TƏTBİQİ*

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Atom quruluşunu təsvir etmək və atom spektrlərini öyrənmək üçün yüngül və ağır atomlara müxtəlif cütləşmə sxemləri tətbiq olunur. jj –cütləşmə, spin-orbit qarşılıqlı təsirin elektrostatik qarşılıqlı təsir üzərində üstünlük təşkil edən ağır atomlar üçün vacibdir. Burada, bütün mümkün olan mikrovəziyyətlərin analizindən jj termləri və J səviyyələri mümkün olan qeyri-ekvivalent $f^n f^{n'}$ *(n & n' = 1-2) elektronlar üçün müəyyən edilmişdir. Təyyin olunmuş jj termlər* $\left[\left(j_1, j_2, j_3, \ldots \ldots j_N\right)_J\right]$ *şəklində işarə edilmişdir.*

Açar sözlər: *jj –cütləşmə, qeyri-ekvivalent, atom spektrləri*