LS, *JK*, and *jj* Atomic Spectroscopic Terms and Spectroscopic Terms for small molecules

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jj coupling

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X Brazilian Meeting on Rare Earths, BMRE-2024
III Workshop on Theoretical Bioinorganic Chemistry, WTBC-2024
September 12th - 15th, 2024

References

Advanced books

- Harris, D. C.; Bertolucci, M. D. *Symmetry and Spectroscopy*, Oxford, 1978

- Cowan, R. D. *The Theory of Atomic Structure and Spectra*, University of California Press, 1981.

- Bernath, P. F. *Spectra of Atoms and Molecules*, 3rd, ed., Oxford University Press, 2016.

Articles on *jj* coupling

- Gauerke, E. S. J.; Campbell, M. L. A Simple, Systematic Method for Determining J Levels for jj Coupling, *J. Chem. Educ.* **1994**, *71*, 457-463. DOI: 10.1021/ed071p457

- Haigh, C. W. The Theory of Atomic Spectroscopy: jj Coupling, Intermediate Coupling, and Configuration Interaction, *J. Chem. Educ.* **1995**, *72*, 206-210. DOI: 10.1021/ed072p206

- Campbell, M. L. Rules for Determining the Ground State of a *j-j* Coupled Atom, *J. Chem. Educ.* **1998**, *75*, 1339-1340. DOI: 10.1021/ed075p1339

Articles on *jj* coupling

- Orofino, H.; Faria, R. B. Obtaining the Electron Angular Momentum Coupling Spectroscopic Terms, jj, *J. Chem. Educ.* **2010**, *87*, 1451-1454. DOI: 10.1021/ed1004245

LS and *jj* comparison

- Dias, L. A. L.; Cardozo, T. M.; Faria, R. B. The Role of jj Coupling on the Energy Levels of Heavy Atoms, *Quim. Nova* **2025**, *48*(1):e-20250006, 1-7. DOI: 10.21577/0100-4042.20250006

Site for energy levels and line spectra of elements and ions

NIST, National Institute of Standard and Technology, Atomic Spectra Database, https://www.nist.gov/pml/atomic-spectra-database

jj coupling

jj terms for lead

ASD Data — Lines Levels — Information — List of Spectra, Ground States & Ionization Energies, Bibliography, Help

NIST National Institute of Standards and Technology — Physical Meas. Laboratory

NIST Atomic Spectra Database Levels Data

Example of how to reference these results:
Kramida, A., Ralchenko, Yu., Reader, J., and NIST ASD Team (2021). *NIST Atomic Spectra Database* (ver. 5.9), [Online]. Available: https://physics.nist.gov/asd [2022, June 1]. National Institute of Standards and Technology, Gaithersburg, MD. DOI: https://doi.org/10.18434/T4W30F

BibTex Citation (new window)

Pb I 136 Levels Found

Z = 82, Pb isoelectronic sequence

Some data for neutral and singly-charged ions are available in the Handbook of Basic Atomic Spectroscopic Data

Primary data source

Query NIST Bibliographic Database for **Pb I** (new window)

Wood & Andrew 1968, Moore 1958

Newer data on some energy levels exists in the literature. Consult the current bibliography for up-to-date information. Alternate LS-coupling designations for some of the levels are from Moore 1958. Some energy levels that were not observed by Wood & Andrew are quoted from Moore 1958. Their J_1l-coupling designations are tentatively assigned based on similarities along series. The ionization limit is from Dembczyński et al. 1994.

Literature on Pb I Energy Levels

jj terms for lead

Configuration	Term	*J*	*g*	Level (cm^{-1})
$6s^2 6p^2$	$(^1/_2, ^1/_2)$	0	1	0.000
$6s^2 6p^2$	$(^3/_2, ^1/_2)$	1	3	7 819.2626
		2	5	10 650.3271
$6s^2 6p^2$	$(^3/_2, ^3/_2)$	2	5	21 457.7982
		0	1	29 466.8303
$6s^2 6p7s$	$(^1/_2, ^1/_2)^\circ$	0	1	*34 959.9084*
		1	3	*35 287.2244*
$6s^2 6p7p$	$(^1/_2, ^1/_2)$	1	3	42 918.6434
		0	1	44 400.8898
$6s^2 6p7p$	$(^1/_2, ^3/_2)$	1	3	44 674.9859
		2	5	44 809.3636

jj coupling

➢ In the ***jj* coupling** case, the spin-orbit coupling is stronger than the electrostatic interactions (Coulomb interaction) between electrons.

➢ The *jj* coupling is more appropriate for the heavier elements.

jj coupling

It is based on the

- total angular moment of the electrons
- total angular moment of the atom

jj coupling

Quantum numbers

- total angular moment of each electron, j
- total angular moment of the atom, J

jj coupling

$$(j_1, j_2, j_3, \ldots)_J$$

- j_1, j_2, j_3, ... are the total angular moment quantum numbers for each electron
- J is the total angular moment quantum number for the atom

jj coupling

$$(j_1, j_2, j_3, \ldots)_J$$

➢ For heavy atoms, ℓ and s are no longer good quantum numbers.

➢ We must work only with j quantum numbers.

jj coupling

$$(j_1, j_2, j_3, \ldots)_J$$

➢ It is equivalent to say that, for heavy atoms, there are no s, p, d, f, etc. orbitals any more.

jj coupling - p^2 electronic configuration

Obtaining the *jj* terms for an atom

1. Calculate the possibles *j* values for each electron
2. Determine the possible combinations of *j* the values inside the parenthesis
3. Built the microstates putting the electrons in the "m_j orbitals"
4. Compute all possible M_J values as Σm_j
5. Built the ocorrence table
6. Extract the terms

jj coupling - p^2 electronic configuration

Calculating the possible *j* values for each electron

- Electrons are in a p orbital ⇨ $\ell = 1$
- Spin quantum number of any electron, $s = ½$

- $j = \ell + s, \ell + s - 1, \ell + s - 2, \ldots |\ell - s|$

⇨ *j* for each electron can be 3/2 or 1/2

jj coupling - p^2 electronic configuration

jj terms possibilities

$(3/2, 3/2)_J$

$(3/2, 1/2)_J$

$(1/2, 1/2)_J$

Which are the *J* values?

jj coupling - p^2 electronic configuration

Pauli exclusion principle

If $j_1 = j_2$

then, $m_{j1} \neq m_{j2}$

jj coupling - p^2 electronic configuration

jj terms possibilities

$(3/2, 3/2)_J$

$(3/2, 1/2)_J$

$(1/2, 1/2)_J$

Which are the *J* values?

jj coupling - p^2 electronic configuration

Building the microstates for the term $(3/2, 1/2)_J$

electron 1 ($j = 3/2$)				electron 2 ($j = 1/2$)		
$m_j = -3/2$	$m_j = -1/2$	$m_j = 1/2$	$m_j = 3/2$	$m_j = -1/2$	$m_j = 1/2$	$M_J = \sum m_j$
#				#		-2
#					#	-1
	#			#		-1
	#				#	0
		#		#		0
		#			#	1
			#	#		1
			#		#	2

jj coupling - p^2 electronic configuration

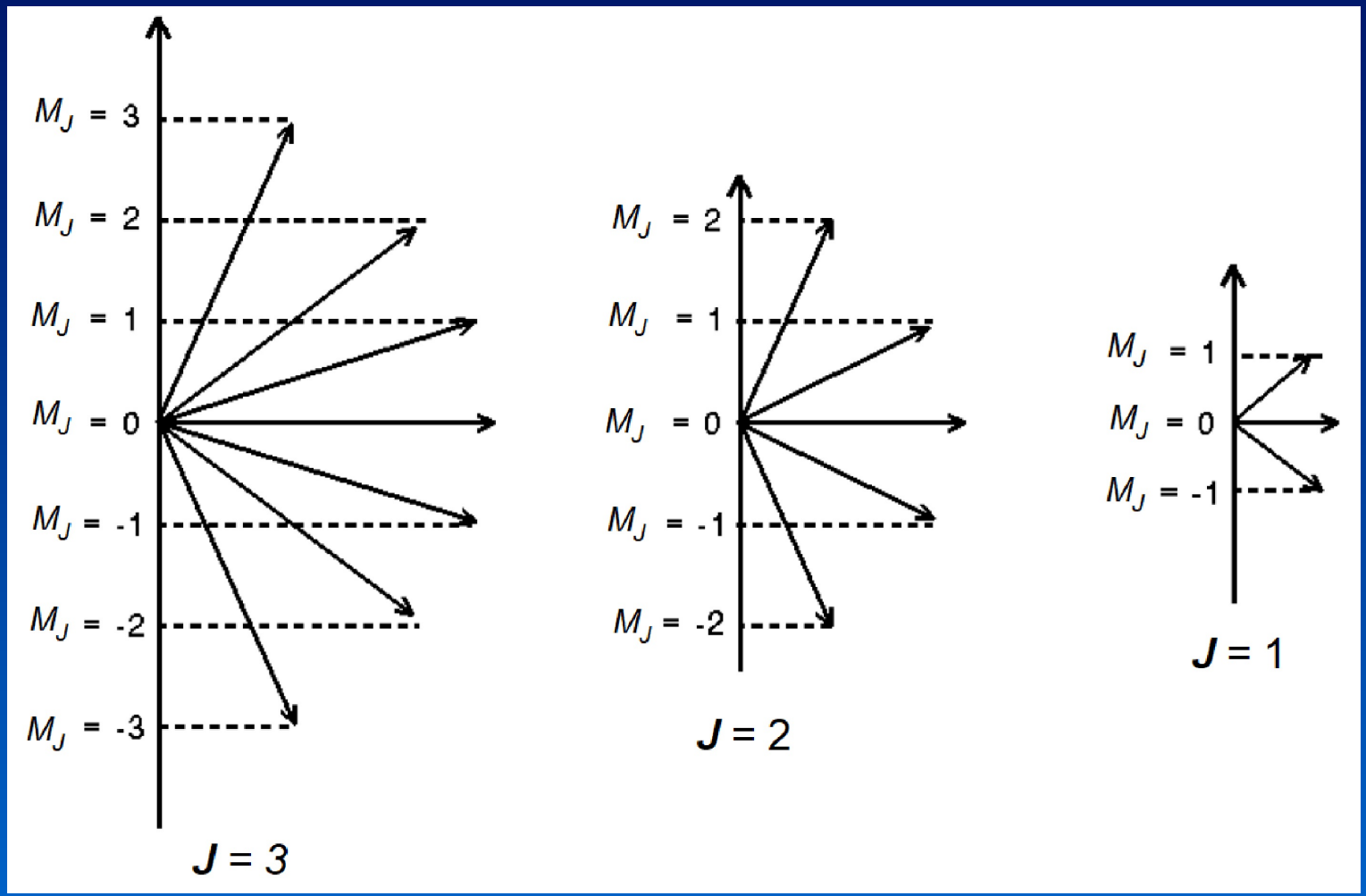
Counting the microstates and obtaining the J values

	counting the microstates	Number of microstates after remove the $(3/2,1/2)_2$ term
$M_J = 2$	1	
$M_J = 1$	2	1
$M_J = 0$	2	1
$M_J = -1$	2	1
$M_J = -2$	1	

$J = 2$ $J = 1$

jj coupling - p^2 electronic configuration

The vector model



jj coupling - p^2 electronic configuration

Term symbols

$(3/2, 3/2)_J$

$(3/2, 1/2)_{2,1}$

$(1/2, 1/2)_J$

Which are the *J* values?

jj coupling - p^2 electronic configuration

Term symbols

$(3/2, 3/2)_J$

$(3/2, 1/2)_{2,1}$

$(1/2, 1/2)_J$

Which are the *J* values?

jj coupling - p^2 electronic configuration

Building the microstates for the term $(3/2, 3/2)_J$

electron 1 ($j = 3/2$)				electron 2 ($j = 3/2$)				
m_j -3/2	m_j -1/2	m_j 1/2	m_j 3/2	m_j -3/2	m_j -1/2	m_j 1/2	m_j 3/2	$M_J = \sum m_j$
#					#			-2
#						#		-1
#							#	0
	#					#		0
	#						#	1
		#					#	2

jj coupling - p^2 electronic configuration

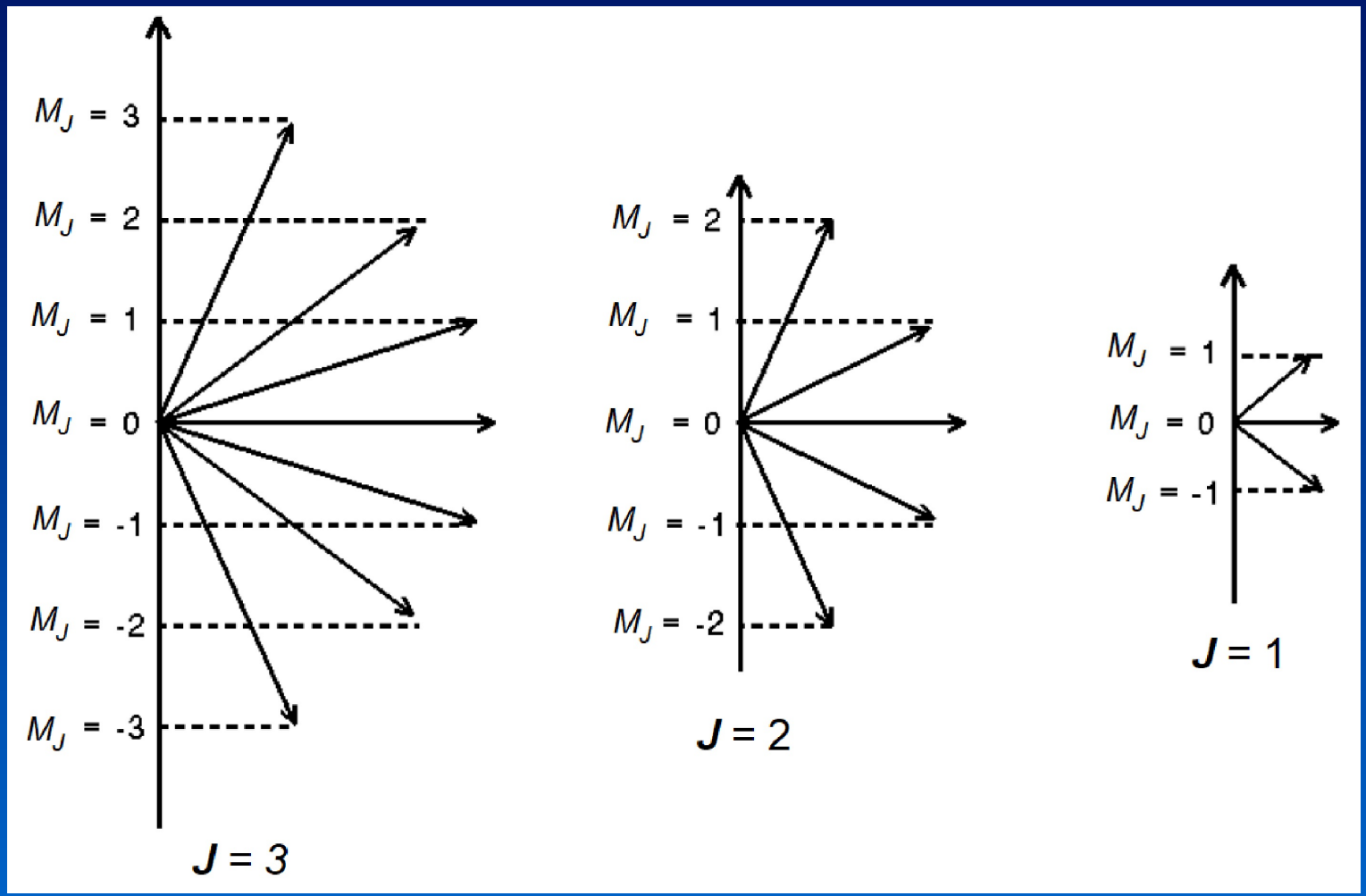
Counting the microstates and obtaining the J values

	counting the microstates	Number of microstates after remove the $(3/2,3/2)_2$ term
$M_J = 2$	1	
$M_J = 1$	1	
$M_J = 0$	2	1
$M_J = -1$	1	
$M_J = -2$	1	

$J = 2$ $J = 0$

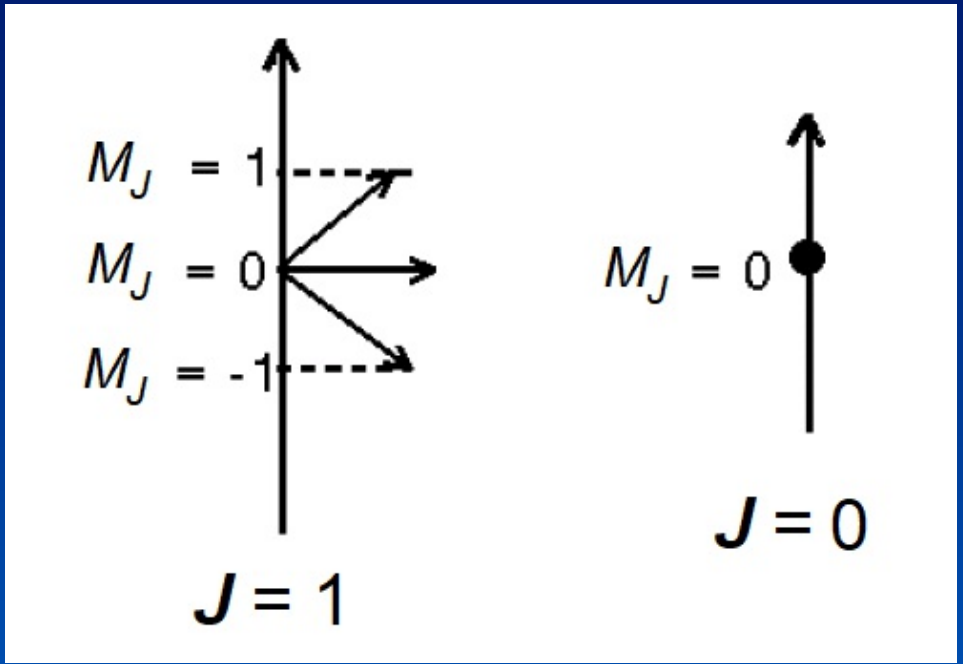
jj coupling - p^2 electronic configuration

The vector model



jj coupling - p^2 electronic configuration

The vector model



jj coupling - p^2 electronic configuration

Term symbols

$(3/2, 3/2)_{2,0}$

$(3/2, 1/2)_{2,1}$

$(1/2, 1/2)_{J}$

Which are the *J* values?

jj coupling - p^2 electronic configuration

Term symbols

$(3/2, 3/2)_{2,0}$

$(3/2, 1/2)_{2,1}$

$(1/2, 1/2)_J$

Which are the *J* values?

jj coupling - p^2 electronic configuration

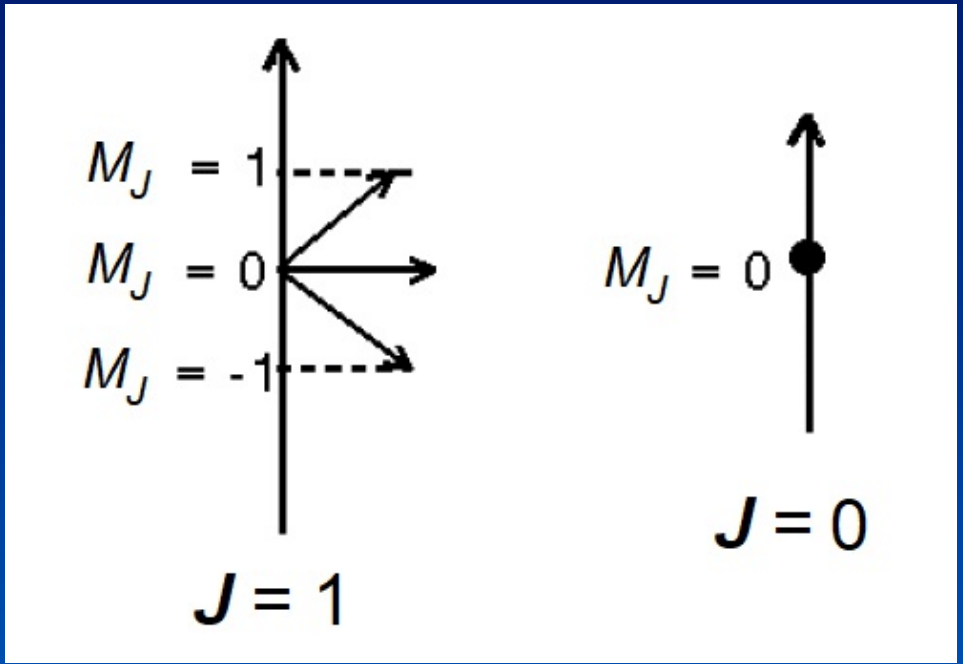
Building the microstates for the term $(1/2, 1/2)_J$

electron 1 ($j = 1/2$)		electron 2 ($j = 1/2$)		
m_j -1/2	m_j 1/2	m_j -1/2	m_j 1/2	$M_J = \sum m_j$
#			#	0

$J = 0$

jj coupling - p^2 electronic configuration

The vector model



jj coupling - p^2 electronic configuration

Term symbols

$(3/2, 3/2)_{2,0}$

$(3/2, 1/2)_{2,1}$

$(1/2, 1/2)_{0}$

jj coupling - p^2 electronic configuration

Final term symbols

$(3/2, 3/2)_{2,0}$

$(3/2, 1/2)_{2,1}$

$(1/2, 1/2)_{0}$

jj coupling - p^2 electronic configuration

Hund's rules

➢ Hund's rules are empirical rules which are valid only for the lowest energy term.

➢ Hund's rules are applied once to determine the lower energy term, and cannot be applied to other terms of higher energy.

jj coupling - p^2 electronic configuration

Hund's rules

1) The term with the lowest set of *j* values inside the parenthesis is the lower energy term.

2) If there is more then one *J* value, the term with the higher *J* value is the lower energy term.

- As a result, the lowest energy term is $(1/2, 1/2)_0$

- The energy sequency of the other terms can be determined by other methods, but not by the use of the Hund's rules

jj terms for lead

Configuration	Term	*J*	*g*	Level (cm^{-1})
$6s^2 6p^2$	$(^1/_2, ^1/_2)$	0	1	0.000
$6s^2 6p^2$	$(^3/_2, ^1/_2)$	1	3	7 819.2626
		2	5	10 650.3271
$6s^2 6p^2$	$(^3/_2, ^3/_2)$	2	5	21 457.7982
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$6s^2 6p7s$	$(^1/_2, ^1/_2)^\circ$	0	1	*34 959.9084*
		1	3	*35 287.2244*
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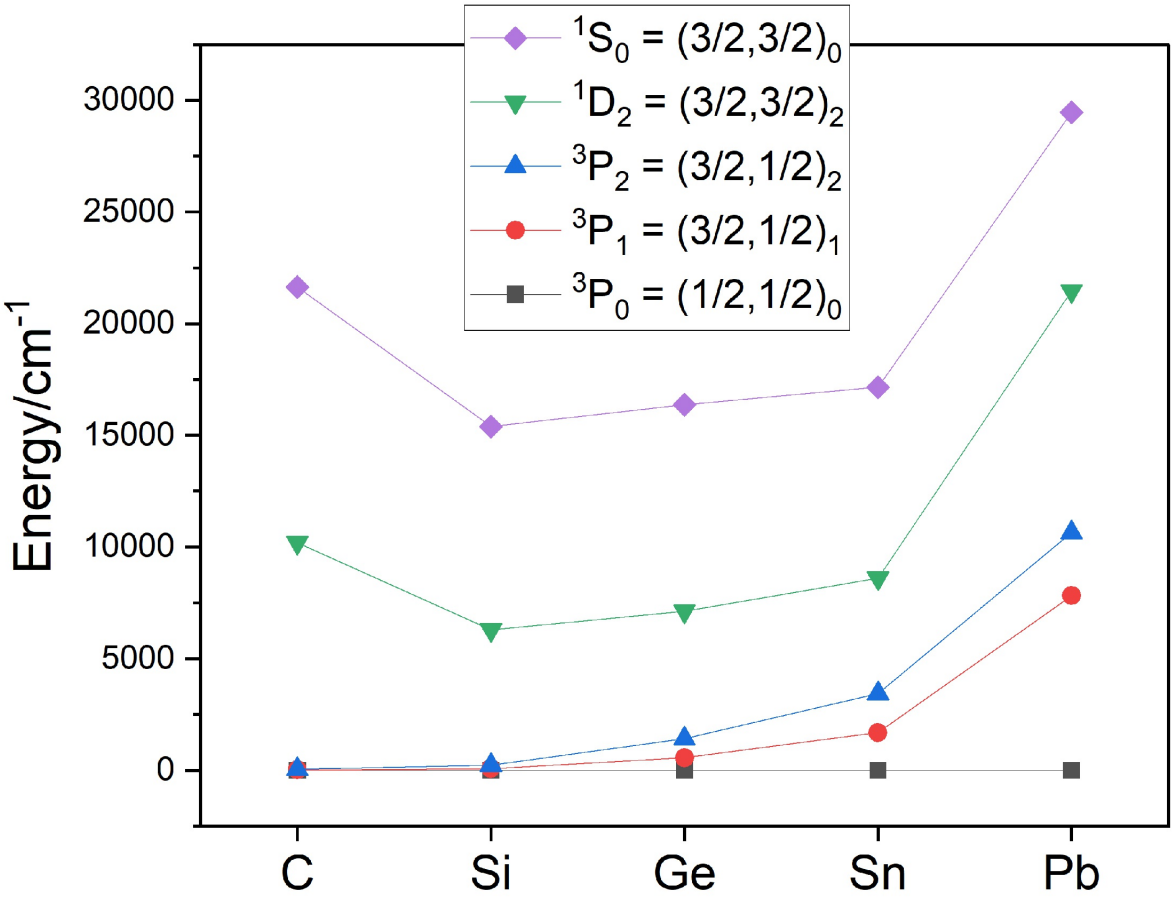
		0	1	44 400.8898
$6s^2 6p7p$	$(^1/_2, ^3/_2)$	1	3	44 674.9859
		2	5	44 809.3636

$(3/2, 3/2)_{2,0}$

$(3/2, 1/2)_{2,1}$

$(1/2, 1/2)_0$

LS and *jj* comparison (p^2)



Dias, L. A. L.; Cardozo, T. M.; Faria, R. B. The Role of jj Coupling on the Energy Levels of Heavy Atoms, *Quim. Nova 48*(1):e-20250006, 1-7 (2025)

jj coupling - p^3 electronic configuration

Calculating the possible *j* values for each electron

- Electrons are in a p orbital ⇨ $\ell = 1$
- Spin quantum number of any electron, $s = ½$

- $j = \ell + s, \ell + s - 1, \ell + s - 2, \ldots |\ell - s|$

⇨ *j* for each electron can be 3/2 or 1/2

jj coupling - p^3 electronic configuration

jj terms possibilities

$(3/2, 3/2, 3/2)_J^\circ$

$(3/2, 3/2, 1/2)_J^\circ$

$(3/2, 1/2, 1/2)_J^\circ$

$(1/2, 1/2, 1/2)_J^\circ$

The parity symbol indicates that the sum of all ℓ is an odd number (p + p + p; 1 + 1 + 1 = 3).

jj coupling - p^3 electronic configuration

jj terms possibilities

$(3/2, 3/2, 3/2)_J^\circ$

$(3/2, 3/2, 1/2)_J^\circ$

$(3/2, 1/2, 1/2)_J^\circ$

$(1/2, 1/2, 1/2)_J^\circ$

Which are the *J* values?

jj coupling - p^3 electronic configuration

Pauli exclusion principle

If $j_1 = j_2$

then, $m_{j1} \neq m_{j2}$

jj coupling - p^3 electronic configuration

jj terms possibilities

$(3/2, 3/2, 3/2)_J^\circ$

$(3/2, 3/2, 1/2)_J^\circ$

$(3/2, 1/2, 1/2)_J^\circ$

$(1/2, 1/2, 1/2)_J^\circ$

Which are the J values?

jj coupling - p^3 electronic configuration

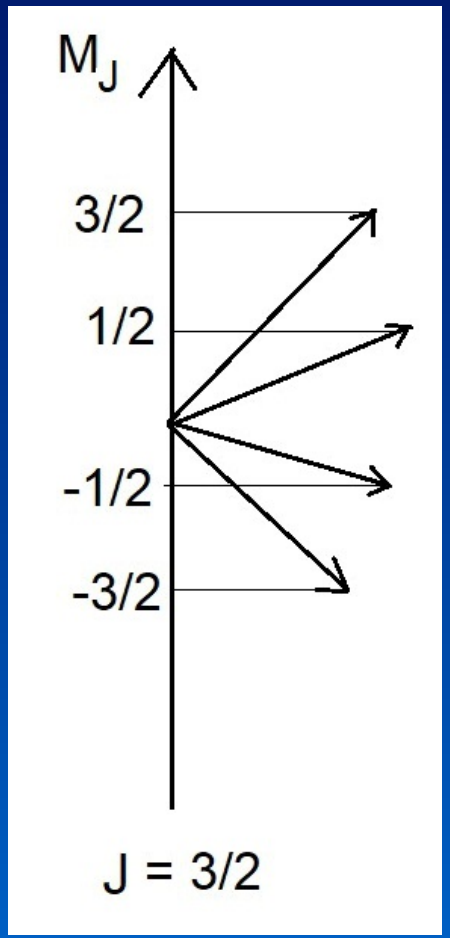
Building the microstates for the term $(3/2, 3/2, 3/2)_J^\circ$

electrons 1, 2 e 3 ($j_1 = j_2 = j_3 = 3/2$)				
m_j -3/2	m_j -1/2	m_j 1/2	m_j 3/2	$M_J = \sum m_j$
#	#	#		-3/2
#	#		#	-1/2
#		#	#	1/2
	#	#	#	3/2

$J = 3/2$

jj coupling - p^3 electronic configuration

The vector model



jj coupling - p^3 electronic configuration

jj terms possibilities

$(3/2, 3/2, 3/2)_{3/2}°$

$(3/2, 3/2, 1/2)_J°$

$(3/2, 1/2, 1/2)_J°$

$(1/2, 1/2, 1/2)_J°$

Which are the *J* values?

jj coupling - p^3 electronic configuration

jj terms possibilities

$(3/2, 3/2, 3/2)_{3/2}°$

$(3/2, 3/2, 1/2)_J°$

$(3/2, 1/2, 1/2)_J°$

$(1/2, 1/2, 1/2)_J°$

Which are the *J* values?

jj coupling - p^3 electronic configuration

electrons 1 and 2 ($j_1 = j_2 = 3/2$)				electron 3 ($j = 1/2$)		
m_j -3/2	m_j -1/2	m_j 1/2	m_j 3/2	m_j -1/2	m_j 1/2	$M_J = \sum m_j$
#	#			#		-5/2
#	#				#	-3/2
#		#		#		-3/2
#		#			#	-1/2
#			#	#		-1/2
#			#		#	1/2
	#	#		#		-1/2
	#	#			#	1/2
	#		#	#		1/2
	#		#		#	3/2
		#	#	#		3/2
		#	#		#	5/2

Microstates for the term $(3/2, 3/2, 1/2)_J°$

jj coupling - p^3 electronic configuration

Counting the microstates and obtaining the J values

	number of microstates	number of microstates after remove the term $(3/2,3/2,1/2)_{5/2}$	number of microstates after remove the term $(3/2,3/2,1/2)_{3/2}$
$M_J = 5/2$	1		
$M_J = 3/2$	2	1	
$M_J = 1/2$	3	2	1
$M_J = -1/2$	3	2	1
$M_J = -3/2$	2	1	
$M_J = -5/2$	1		

$J = 5/2$ $J = 3/2$ $J = 1/2$

jj coupling - p^3 electronic configuration

jj terms possibilities

$(3/2, 3/2, 3/2)_{3/2}°$

$(3/2, 3/2, 1/2)_{5/2,3/2,1/2}°$

$(3/2, 1/2, 1/2)_{J}°$

$(1/2, 1/2, 1/2)_{J}°$

Which are the *J* values?

jj coupling - p^3 electronic configuration

jj terms possibilities

$(3/2, 3/2, 3/2)_{3/2}°$

$(3/2, 3/2, 1/2)_{5/2,3/2,1/2}°$

$(3/2, 1/2, 1/2)_J°$

$(1/2, 1/2, 1/2)_J°$

Which are the *J* values?

jj coupling - p^3 electronic configuration

Building the microstates for the term $(3/2, 1/2, 1/2)_J^\circ$

electron 1 ($j_1 = 3/2$)				electrons 2 and 3 ($j_2 = j_3 = 1/2$)		
m_j -3/2	m_j -1/2	m_j 1/2	m_j 3/2	m_j -1/2	m_j 1/2	$M_J = \sum m_j$
#				#	#	-3/2
	#			#	#	-1/2
		#		#	#	1/2
			#	#	#	3/2

$J = 3/2$

jj coupling - p^3 electronic configuration

jj terms possibilities

$(3/2, 3/2, 3/2)_{3/2}°$

$(3/2, 3/2, 1/2)_{5/2,3/2,1/2}°$

$(3/2, 1/2, 1/2)_{3/2}°$

$(1/2, 1/2, 1/2)_{J}°$

Which are the *J* values?

jj coupling - p^3 electronic configuration

jj terms possibilities

$(3/2, 3/2, 3/2)_{3/2}$°

$(3/2, 3/2, 1/2)_{5/2,3/2,1/2}$°

$(3/2, 1/2, 1/2)_{3/2}$°

$(1/2, 1/2, 1/2)_J$°

It is not possible.

Pauli exclusion principle

If $j_1 = j_2$

then, $m_{j1} \neq m_{j2}$

jj coupling - p^3 electronic configuration

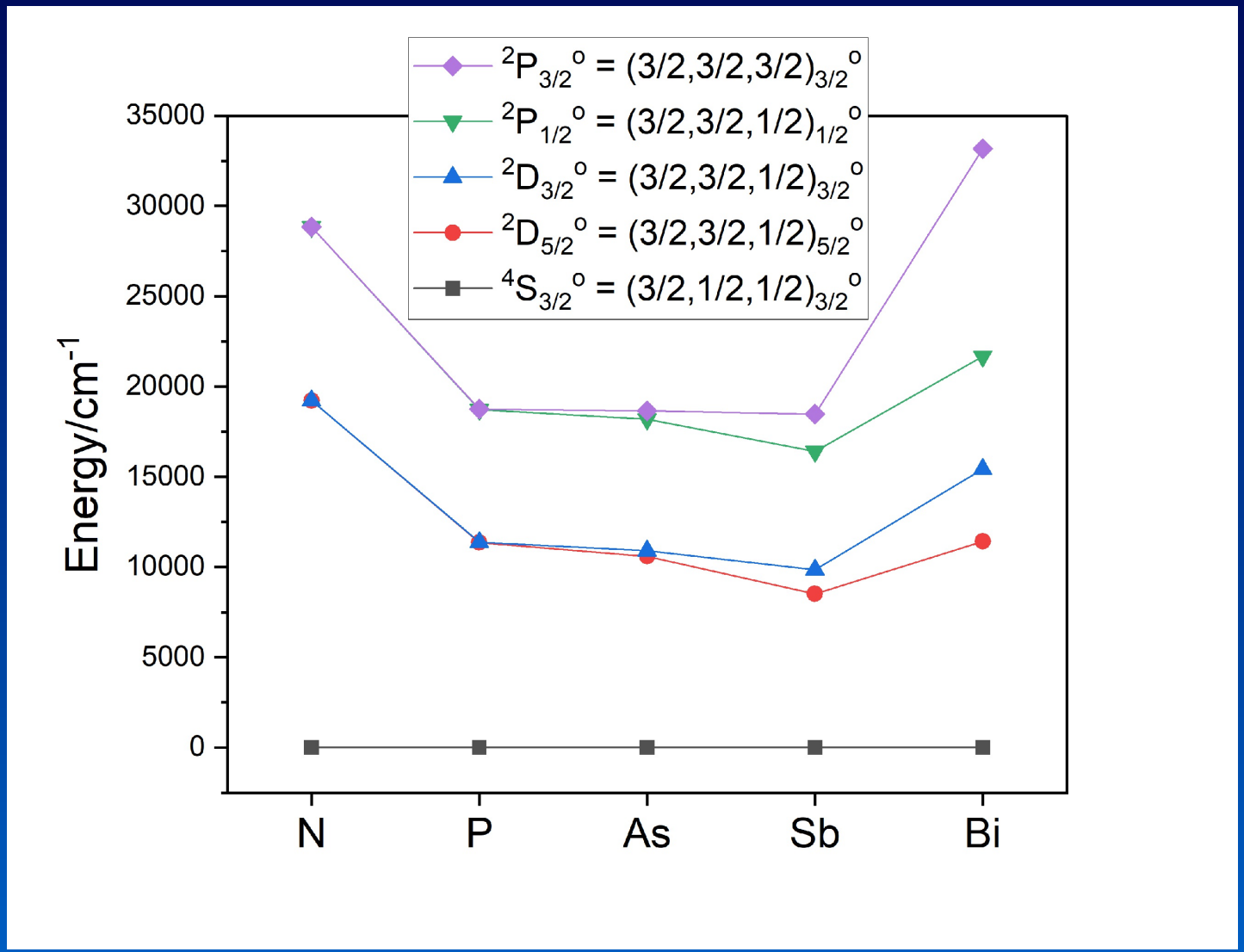
Final term symbols

$(3/2, 3/2, 3/2)_{3/2}^{\circ}$

$(3/2, 3/2, 1/2)_{5/2,3/2,1/2}^{\circ}$

$(3/2, 1/2, 1/2)_{3/2}^{\circ}$

LS and *jj* comparison (p^3)



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jj coupling

s^1	$(1/2)_{1/2}$		
s^2	$(1/2,1/2)_0$		
p^1	$(3/2)_{3/2}^o$	$(1/2)_{1/2}^o$	
p^2	$(3/2, 3/2)_{2,0}$	$(3/2, 1/2)_{2,1}$	$(1/2, 1/2)_0$
p^3	$(3/2, 3/2, 3/2)_{3/2}^o$	$(3/2, 3/2, 1/2)_{5/2, 3/2, 1/2}^o$	$(3/2, 1/2, 1/2)_{3/2}^o$
p^4	$(3/2, 3/2, 3/2, 3/2)_0$	$(3/2, 3/2, 3/2, 1/2)_{2,1}$	$(3/2, 3/2, 1/2, 1/2)_{2,0}$
p^5	$(3/2, 3/2, 3/2, 3/2, 1/2)_{1/2}^o$		
	$(3/2, 3/2, 3/2, 1/2, 1/2)_{3/2}^o$		
p^6	$(3/2, 3/2, 3/2, 3/2, 1/2, 1/2)_0$		

jj coupling - non equivalent electrons

The case s^1p^1

Calculating the possible *j* values for each electron

- Electron in the s orbital ⇨ $\ell = 0$
- Spin quantum number of any electron, $s = ½$

- $j = \ell + s, \ell + s - 1, \ell + s - 2, \ldots |\ell - s|$

⇨ *j* for the electron in the orbital s can be only 1/2

jj coupling - non equivalent electrons

The case s^1p^1

Calculating the possible *j* values for each electron

- Electron in the p orbital ⇨ $\ell = 1$
- Spin quantum number of any electron, $s = ½$

- $j = \ell + s, \ell + s - 1, \ell + s - 2, \ldots |\ell - s|$

⇨ *j* values for the electron in the p orbital can be 3/2 or 1/2

jj coupling - non equivalent electrons

jj terms possibilities for the case s^1p^1

$(p{:}3/2;\ s{:}1/2)_J^\circ$

$(p{:}1/2;\ s{:}1/2)_J^\circ$

The parity symbol indicates that the sum of all ℓ is an odd number (s + p; 0 + 1= 1).

jj coupling - case s^1p^1

jj terms possibilities

$(p{:}3/2;\ s{:}1/2)_J°$

$(p{:}1/2;\ s{:}1/2)_J°$

Which are the *J* values?

jj coupling - case s^1p^1

Building the microstates for the term $(p:3/2; s:1/2)_{J^\circ}$

electron 1 ($j = 3/2$)				electron 2 ($j = 1/2$)		
$m_j = -3/2$	$m_j = -1/2$	$m_j = 1/2$	$m_j = 3/2$	$m_j = -1/2$	$m_j = 1/2$	$M_J = \sum m_j$
#				#		-2
#					#	-1
	#			#		-1
	#				#	0
		#		#		0
		#			#	1
			#	#		1
			#		#	2

jj coupling - case s^1p^1

Counting the microstates and obtaining the J values

	number of microstates	number of microstates after remove the term $(p:3/2; s:1/2)_2$
$M_J = 2$	1	
$M_J = 1$	2	1
$M_J = 0$	2	1
$M_J = -1$	2	1
$M_J = -2$	1	

$J = 2$ $J = 1$

jj coupling - case s^1p^1

jj terms possibilities

$(p{:}3/2;\ s{:}1/2)_{2,1}°$

$(p{:}1/2;\ s{:}1/2)_{J}°$

Which are the *J* values?

jj coupling - case s^1p^1

jj terms possibilities

$(p{:}3/2;\ s{:}1/2)_{2,1}°$

$(p{:}1/2;\ s{:}1/2)_{J}°$

Which are the *J* values?

jj coupling - case s^1p^1

Building the microstates for the term (p:1/2; s:1/2) $_J$°

electron 1 (j = 1/2)		electron 2 (j = 1/2)		
m_j -1/2	m_j 1/2	m_j -1/2	m_j 1/2	$M_J = \sum m_j$
#		#		-1
#			#	0
	#	#		0
	#		#	1

jj coupling - case s^1p^1

Counting the microstates and obtaining the J values

	number of microstates	number of microstates after remove the term $(p:1/2; s:1/2)_1$
$M_J = 1$	1	
$M_J = 0$	2	1
$M_J = -1$	1	

$J = 1$ $J = 0$

jj coupling - case s^1p^1

jj terms possibilities

$(p:3/2;\ s:1/2)_{2,1}^{\circ}$

$(p:1/2;\ s:1/2)_{1,0}^{\circ}$

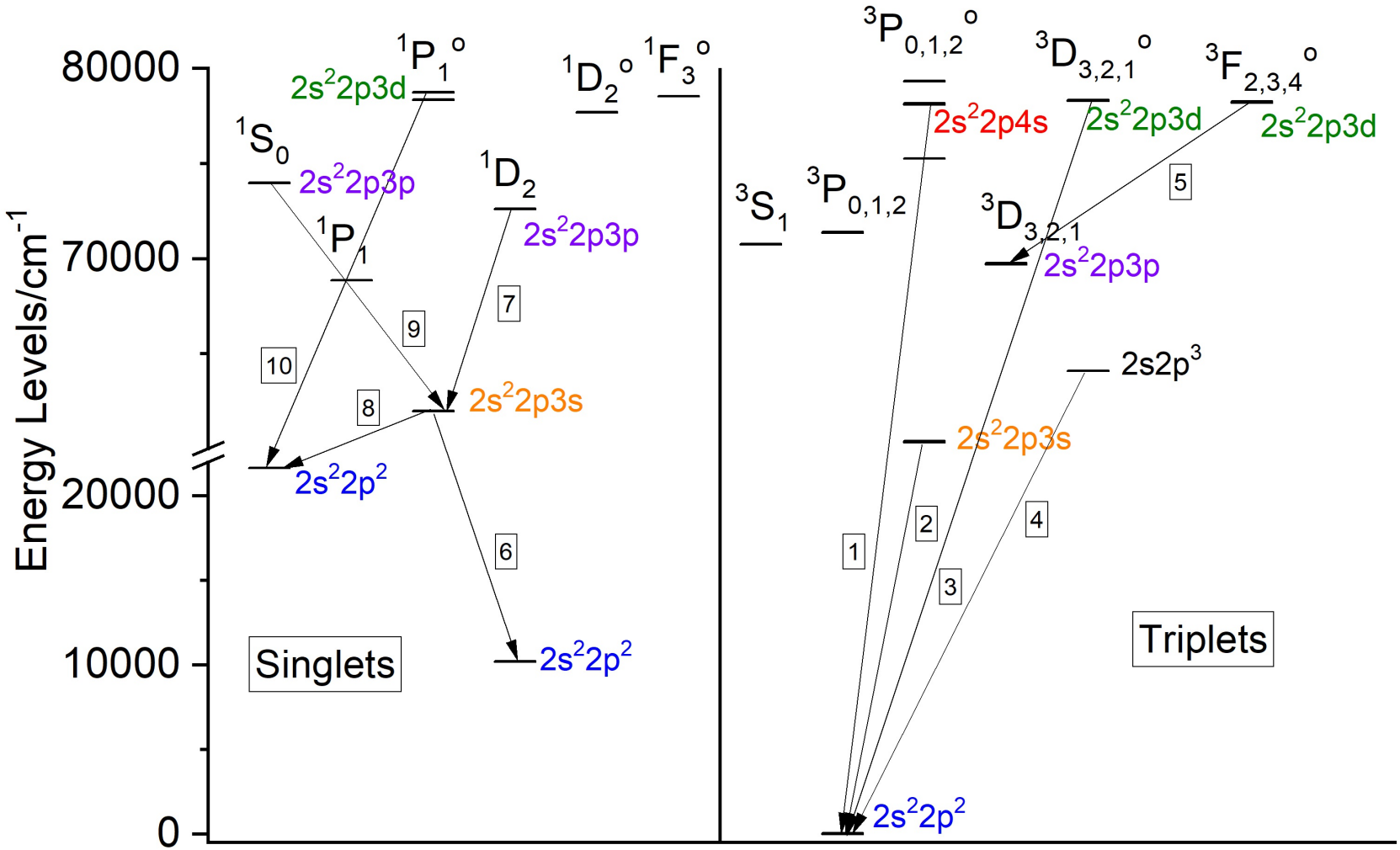
jj coupling - non equivalent electrons

$ns^1n's^1$	$(1/2,1/2)_{1,0}$
s^1p^1	$(3/2;1/2)_{2,1}^{o}$ $(1/2;1/2)_{1,0}^{o}$
s^1p^3	$(3/2,3/2,3/2;1/2)_{2,1}$ $(3/2,3/2,1/2;1/2)_{3,2(2),1(2),0}$ $(3/2,1/2,1/2;1/2)_{2,1}$
$np^1n'p^1$	$(3/2,3/2)_{3,2,1,0}$ $(3/2,1/2)_{2,1}$ $(1/2,1/2)_{1,0}$
s^1d^1	$(5/2;1/2)_{3,2}$ $(3/2;1/2)_{2,1}$
s^1d^2	$(5/2,5/2;1/2)_{9/2,7/2,5/2,3/2,1/2}$ $(5/2,3/2;1/2)_{9/2,2(7/2),2(5/2),2(3/2),1/2}$ $(3/2,3/2;1/2)_{5/2,3/2,1/2}$
$s^1p^1d^1$	$(5/2;3/2;1/2)_{9/2,2(7/2),2(5/2),2(3/2),1/2}^{o}$ $(5/2;1/2;1/2)_{5/2}^{o}$, $(3/2;3/2;1/2)_{7/2,2(5/2),2(3/2),2(1/2)}^{o}$, $(3/2;1/2;1/2)_{3/2}^{o}$
p^1d^1	$(5/2;3/2)_{4,3,2,1}^{o}$ $(5/2;1/2)_{3,2}^{o}$ $(3/2;3/2)_{3,2,1,0}^{o}$ $(3/2;1/2)_{2,1}^{o}$
$nd^1n'd^1$	$(5/2,5/2)_{5,4,3,2,1,0}$ $(5/2,3/2)_{4,3,2,1}$ $(3/2,3/2)_{3,2,1,0}$

Selection Rules
Electric dipole allowed electronic transitions

LS coupling	*jj* coupling
$T \leftrightarrow T^{\circ}$	$T \leftrightarrow T^{\circ}$
$\Delta S = 0$	
$\Delta L = 0, \pm 1$	
$\Delta J = 0, \pm 1$ ($0 \leftrightarrow 0$ forbiden)	$\Delta J = 0, \pm 1$ ($0 \leftrightarrow 0$ forbiden)

Carbon emission spectra (C I) - persistent lines*



*Sansonetti, J. E.; Martin, W. C. *J. Phys. Chem. Ref. Data* **2005**, *34*, 1559-2259

Selection Rules
Electric dipole allowed electronic transitions

LS coupling - carbon is a light element

T $\leftrightarrow$ T° (no "vertical" transitions)

$\Delta S = 0$ (no mixing between singlets and triplets)

$\Delta L = 0, \pm 1$

$\Delta J = 0, \pm 1$ ($0 \leftrightarrow 0$ not allowed)

Electric dipole allowed electronic transitions for carbon triplet ↔ triplet

[1] 128.03330 nm $2s^2\ 2p^1\ 4s^1\ (^3P_2°) \rightarrow 2s^2\ 2p^2\ (^3P_2)$ $\Delta J = 0$ $\Delta L = 0$

[2] Six lines very close

165.8121 nm	$2s^2\ 2p^1\ 3s^1\ (^3P_1°) \rightarrow 2s^2\ 2p^2\ (^3P_2)$	$\Delta J = +1$	$\Delta L = 0$
165.7907 nm	$2s^2\ 2p^1\ 3s^1\ (^3P_0°) \rightarrow 2s^2\ 2p^2\ (^3P_1)$	$\Delta J = +1$	$\Delta L = 0$
165.7379 nm	$2s^2\ 2p^1\ 3s^1\ (^3P_1°) \rightarrow 2s^2\ 2p^2\ (^3P_1)$	$\Delta J = 0$	$\Delta L = 0$
165.7008 nm	$2s^2\ 2p^1\ 3s^1\ (^3P_2°) \rightarrow 2s^2\ 2p^2\ (^3P_2)$	$\Delta J = 0$	$\Delta L = 0$
165.6928 nm	$2s^2\ 2p^1\ 3s^1\ (^3P_1°) \rightarrow 2s^2\ 2p^2\ (^3P_0)$	$\Delta J = -1$	$\Delta L = 0$
165.6267 nm	$2s^2\ 2p^1\ 3s^1\ (^3P_2°) \rightarrow 2s^2\ 2p^2\ (^3P_1)$	$\Delta J = -1$	$\Delta L = 0$

[3] Four lines very close

127.75497 nm	$2s^2\ 2p^1\ 3d^1\ (^3D_3°) \rightarrow 2s^2\ 2p^2\ (^3P_2)$	$\Delta J = -1$	$\Delta L = -1$
127.75131 nm	$2s^2\ 2p^1\ 3d^1\ (^3D_1°) \rightarrow 2s^2\ 2p^2\ (^3P_1)$	$\Delta J = 0$	$\Delta L = -1$
127.72824 nm	$2s^2\ 2p^1\ 3d^1\ (^3D_2°) \rightarrow 2s^2\ 2p^2\ (^3P_1)$	$\Delta J = -1$	$\Delta L = -1$
127.72453 nm	$2s^2\ 2p^1\ 3d^1\ (^3D_1°) \rightarrow 2s^2\ 2p^2\ (^3P_0)$	$\Delta J = -1$	$\Delta L = -1$

Electric dipole allowed electronic transitions for carbon triplet ↔ triplet

[4] three lines very close

156.1438 nm	$2s^2\ 2p^3\ (^3D_3°) \rightarrow 2s^2\ 2p^2\ (^3P_2)$	$\Delta J = -1$	$\Delta L = -1$
156.0709 nm	$2s^2\ 2p^3\ (^3D_1°) \rightarrow 2s^2\ 2p^2\ (^3P_1)$	$\Delta J = 0$	$\Delta L = -1$
156.0682 nm	$2s^2\ 2p^3\ (^3D_2°) \rightarrow 2s^2\ 2p^2\ (^3P_1)$	$\Delta J = -1$	$\Delta L = -1$

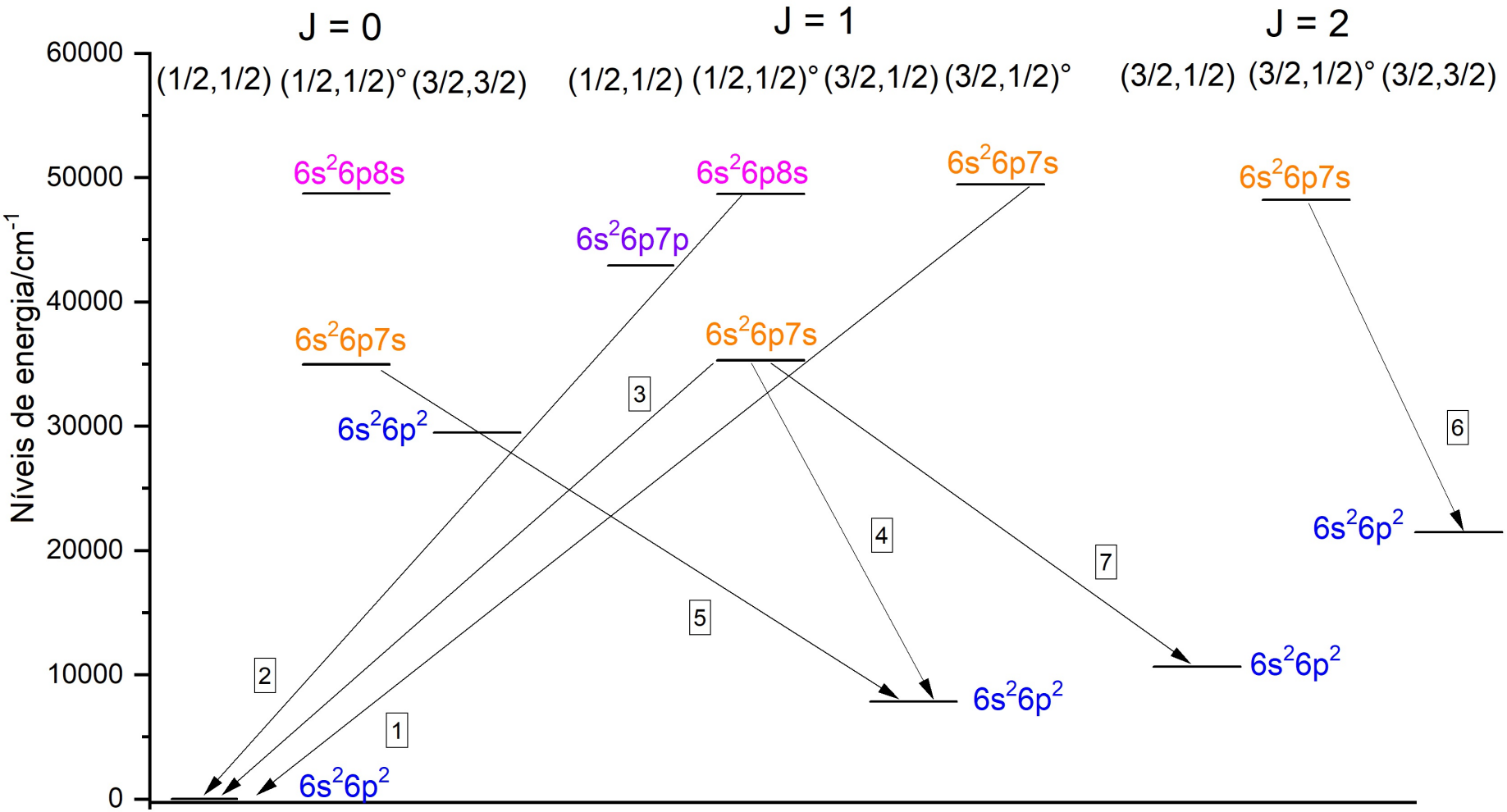
[5] two lines very close

117.5476 nm	$2s^2\ 2p^1\ 3d^1\ (^3F_3°) \rightarrow 2s^2\ 2p^1\ 3p^1\ (^3D_2)$	$\Delta J = -1$	$\Delta L = -1$
117.5332 nm	$2s^2\ 2p^1\ 3d^1\ (^3F_4°) \rightarrow 2s^2\ 2p^1\ 3p^1\ (^3D_3)$	$\Delta J = -1$	$\Delta L = -1$

Electric dipole allowed electronic transitions for carbon singlet ↔ singlet

[6] 193.0906 nm	$2s^2\ 2p^1\ 3s^1\ (^1P_1°) \rightarrow 2s^2\ 2p^2\ (^1D_2)$	$\Delta J = +1$	$\Delta L = +1$
[7] 940.573 nm	$2s^2\ 2p^1\ 3p^1\ (^1D_2) \rightarrow 2s^2\ 2p^1\ 3s^1\ (^1P_1°)$	$\Delta J = -1$	$\Delta L = -1$
[8] 247.8561 nm	$2s^2\ 2p^1\ 3s^1\ (^1P_1°) \rightarrow 2s^2\ 2p^2\ (^1S_0)$	$\Delta J = -1$	$\Delta L = -1$
[9] 833.515 nm	$2s^2\ 2p^1\ 3p^1\ (^1S_0) \rightarrow 2s^2\ 2p^1\ 3s^1\ (^1P_1°)$	$\Delta J = -1$	$\Delta L = +1$
[10] 175.1827 nm	$2s^2\ 2p^1\ 3d^1\ (^1P_1°) \rightarrow 2s^2\ 2p^2\ (^1S_0)$	$\Delta J = -1$	$\Delta L = -1$

Lead emission spectra (Pb I) - persistent lines*



*Sansonetti, J. E.; Martin, W. C. *J. Phys. Chem. Ref. Data* **2005**, *34*, 1559-2259

Selection Rules
Electric dipole allowed electronic transitions

jj coupling - lead is a heavy element

T $\leftrightarrow$ T° (no "vertical" transitions)

$\Delta J = 0, \pm 1$ ($0 \leftrightarrow 0$ not allowed)

Electric dipole allowed electronic transitions for lead

[1] 202.2016 nm $6s^2\ 6p\ 7s\ (3/2,1/2)_1^\circ \rightarrow 6s^2\ 6p^2\ (1/2,1/2)_0$ $\Delta J = -1$

[2] 205.3284 nm $6s^2\ 6p\ 8s\ (1/2,1/2)_1^\circ \rightarrow 6s^2\ 6p^2\ (1/2,1/2)_0$ $\Delta J = -1$

[3] 283.3053 nm $6s^2\ 6p\ 7s\ (1/2,1/2)_1^\circ \rightarrow 6s^2\ 6p^2\ (1/2,1/2)_0$ $\Delta J = -1$

[4] 363.9568 nm $6s^2\ 6p\ 7s\ (1/2,1/2)_1^\circ \rightarrow 6s^2\ 6p^2\ (3/2,1/2)_1$ $\Delta J = 0$

[5] 368.3462 nm $6s^2\ 6p\ 7s\ (1/2,1/2)_0^\circ \rightarrow 6s^2\ 6p^2\ (3/2,1/2)_1$ $\Delta J = +1$

[6] 373.9935 nm $6s^2\ 6p\ 7s\ (3/2,1/2)_2^\circ \rightarrow 6s^2\ 6p^2\ (3/2,3/2)_2$ $\Delta J = 0$

[7] 405.7807 nm $6s^2\ 6p\ 7s\ (1/2,1/2)_1^\circ \rightarrow 6s^2\ 6p^2\ (3/2,1/2)_2$ $\Delta J = +1$

Electric dipole allowed electronic transitions for lead

[1] 202.2016 nm $6p_{3/2}\,7s_{1/2}\,(3/2,1/2)_1^\circ \rightarrow 6p_{1/2}^2\,(1/2,1/2)_0$ $\Delta J = -1$

[2] 205.3284 nm $6p_{1/2}\,8s_{1/2}\,(1/2,1/2)_1^\circ \rightarrow 6p_{1/2}^2\,(1/2,1/2)_0$ $\Delta J = -1$

[3] 283.3053 nm $6p_{1/2}\,7s_{1/2}\,(1/2,1/2)_1^\circ \rightarrow 6p_{1/2}^2\,(1/2,1/2)_0$ $\Delta J = -1$

[4] 363.9568 nm $6p_{1/2}\,7s_{1/2}\,(1/2,1/2)_1^\circ \rightarrow 6p_{1/2}\,6p_{3/2}\,(3/2,1/2)_1$ $\Delta J = 0$

[5] 368.3462 nm $6p_{1/2}\,7s_{1/2}\,(1/2,1/2)_0^\circ \rightarrow 6p_{1/2}\,6p_{3/2}\,(3/2,1/2)_1$ $\Delta J = +1$

[6] 373.9935 nm $6p_{3/2}\,7s_{1/2}\,(3/2,1/2)_2^\circ \rightarrow 6p_{3/2}^2\,(3/2,3/2)_2$ $\Delta J = 0$

[7] 405.7807 nm $6p_{1/2}\,7s_{1/2}\,(1/2,1/2)_1^\circ \rightarrow 6p_{1/2}p_{3/2}\,(3/2,1/2)_2$ $\Delta J = +1$