Termos Espectroscópicos Acoplamento *JK*

Roberto B. Faria

faria@iq.ufrj.br

www.iq.ufrj.br/~faria

Instituto de Química

Universidade Federal do Rio de Janeiro

Acoplamento *JK*

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Referência

- Cowan, R. D. *The theory of atomic structure and spectra*, University of California Press, 1981.

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Termos *JK* para o carbono

DATA INFORMATION

LINES LEVELS 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

C I 435 Levels Found
Z = 6, C isoelectronic sequence

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, October 15]. National Institute of Standards and Technology, Gaithersburg, MD. DOI: <https://doi.org/10.18434/T4W30F>
[BibTex Citation](#) (new window)

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 C I](#) (new window)
[Hris & Kramida 2017](#) [Literature on C I Energy Levels](#)

Termos JK para o carbono

Configuration	Term	J	g	Level (cm^{-1})
$2s^2 2p^2$	3P	0	1	0.0000000
		1	3	16.4167130
		2	5	43.4134567
$2s^2 2p^2$	1D	2	5	10 192.657
$2s^2 2p^2$	1S	0	1	21 648.030
$2s 2p^3$	$^5S^\circ$	2	5	33 735.121
$2s^2 2p 3s$	$^3P^\circ$	0	1	60 333.4476
		1	3	60 352.6584
		2	5	60 393.1693
$2s^2 2p 3s$	$^1P^\circ$	1	3	61 981.83211
$2s 2p^3$	$^3D^\circ$	3	7	64 086.96961
		1	3	64 089.8990
		2	5	64 090.99351

Termos JK para o carbono

$2s^2 2p(2P^{\circ}_{1/2}) 4f$	$2[5/2]$	3	7	83 919.66322
		2	5	83 919.77375
$2s^2 2p(2P^{\circ}_{1/2}) 4f$	$2[7/2]$	3	7	83 926.22434
		4	9	83 926.42382
$2s^2 2p 4d$	$1F^{\circ}$	3	7	83 947.2231
$2s^2 2p(2P^{\circ}_{3/2}) 4f$	$2[7/2]$	3	7	83 986.22212
		4	9	83 986.4926
$2s^2 2p(2P^{\circ}_{3/2}) 4f$	$2[5/2]$	3	7	84 013.27526
		2	5	84 013.4311
$2s^2 2p(2P^{\circ}_{3/2}) 4f$	$2[9/2]$	5	11	84 015.87795
		4	9	84 016.2748
$2s^2 2p 4d$	$1P^{\circ}$	1	3	84 032.1471
$2s^2 2p(2P^{\circ}_{3/2}) 4f$	$2[3/2]$	1	3	84 036.3320
		2	5	84 036.4454

Acoplamento LS

s^1	${}^2S_{1/2}$
s^2	1S_0
p^1, p^5	${}^2P_{3/2,1/2}^{\circ}$
p^2, p^4	${}^3P_{2,1,0} \quad {}^1D_2 \quad {}^1S_0$
p^3	${}^4S_{3/2}^{\circ} \quad {}^2D_{5/2,3/2}^{\circ} \quad {}^2P_{3/2,1/2}^{\circ}$
p^6	1S_0
d^1, d^9	${}^2D_{5/2,3/2}$
d^2, d^8	${}^3F_{4,3,2} \quad {}^3P_{2,1,0} \quad {}^1G_4 \quad {}^1D_2 \quad {}^1S_0$
d^3, d^7	${}^4F_{9/2,7/2,5/2,3/2} \quad {}^4P_{5/2,3/2,1/2} \quad {}^2H_{11/2,9/2} \quad {}^2G_{9/2,7/2} \quad {}^2F_{7/2,5/2} \quad {}^2D(2)_{5/2,3/2} \quad {}^2P_{3/2,1/2}$
d^4, d^6	${}^5D_{4,3,2,1,0} \quad {}^3H_{6,5,4} \quad {}^3G_{5,4,3} \quad {}^3F(2)_{4,3,2} \quad {}^3D_{3,2,1} \quad {}^3P(2)_{2,1,0} \quad {}^1I_6 \quad {}^1G(2)_4 \quad {}^1F_3 \quad {}^1D(2)_2$ ${}^1S(2)_0$
d^5	${}^6S_{5/2} \quad {}^4G_{11/2,9/2,7/2,5/2} \quad {}^4F_{9/2,7/2,5/2,3/2} \quad {}^4D_{7/2,5/2,3/2,1/2} \quad {}^4P_{5/2,3/2,1/2} \quad {}^2I_{13/2,11/2}$ ${}^2H_{11/2,9/2} \quad {}^2G(2)_{9/2,7/2} \quad {}^2F(2)_{7/2,5/2} \quad {}^2D(3)_{5/2,3/2} \quad {}^2P_{3/2,1/2} \quad {}^2S_{1/2}$
d^{10}	1S_0

Acoplamento LS

s^1	$^2S_{1/2}$
s^2	1S_0
p^1, p^5	$^2P_{3/2,1/2}^{\circ}$
p^2, p^4	$^3P_{2,1,0} \quad ^1D_2 \quad ^1S_0$
p^3	$^4S_{3/2}^{\circ} \quad ^2D_{5/2,3/2}^{\circ} \quad ^2P_{3/2,1/2}^{\circ}$
p^6	1S_0
d^1, d^9	$^2D_{5/2,3/2}$
d^2, d^8	$^3F_{4,3,2} \quad ^3P_{2,1,0} \quad ^1G_4 \quad ^1D_2 \quad ^1S_0$
d^3, d^7	$^4F_{9/2,7/2,5/2,3/2} \quad ^4P_{5/2,3/2,1/2} \quad ^2H_{11/2,9/2} \quad ^2G_{9/2,7/2} \quad ^2F_{7/2,5/2} \quad ^2D(2)_{5/2,3/2} \quad ^2P_{3/2,1/2}$
d^4, d^6	$^5D_{4,3,2,1,0} \quad ^3H_{6,5,4} \quad ^3G_{5,4,3} \quad ^3F(2)_{4,3,2} \quad ^3D_{3,2,1} \quad ^3P(2)_{2,1,0} \quad ^1I_6 \quad ^1G(2)_4 \quad ^1F_3 \quad ^1D(2)_2$ $^1S(2)_0$
d^5	$^6S_{5/2} \quad ^4G_{11/2,9/2,7/2,5/2} \quad ^4F_{9/2,7/2,5/2,3/2} \quad ^4D_{7/2,5/2,3/2,1/2} \quad ^4P_{5/2,3/2,1/2} \quad ^2I_{13/2,11/2}$

Termos JK para o carbono

- É usado para estados excitados envolvendo um elétron em orbitais f ou g
- Os elétrons do caroço interagem pelo acoplamento LS
- A interação com o elétron excitado é independente do spin
- O acoplamento JK considera um novo número quântico, K , calculado pela eq. (1).
- J é calculado pela eq. (2), onde s é o spin do elétron no orbital f ou g ($s = 1/2$)

$$K = J_{\text{caroço}} + l, J_{\text{caroço}} + l - 1, J_{\text{caroço}} + l - 2, \dots, |J_{\text{caroço}} - l| \quad (1)$$

$$J = K + s, K + s - 1, K + s - 2, \dots, |K - s| \quad (2)$$

Termos JK para o carbono

$$^{2S+1}[K]_J$$

A multiplicidade de spin considera apenas o spin do elétron mais externo (f ou g) = $2S+1 = 2(1/2) + 1 = 2$

Como resultado, todos os termos serão dubletos

$$^2[K]_J$$

Termos JK para o carbono

$${}^2[K]_J$$

Configuração eletrônica: $2s^2 2p^1 4f^1$

Termos da configuração do caroço $2s^2 2p^1$: ${}^2P_{3/2,1/2}^\circ$

Escolhendo o termo ${}^2P_{1/2}^\circ$ ($J_{\text{caroço}} = 1/2$)

$$2s^2 2p^1 ({}^2P_{1/2}^\circ) 4f^1$$

$$K = J_{\text{caroço}} + l, J_{\text{caroço}} + l - 1, J_{\text{caroço}} + l - 2, \dots, |J_{\text{caroço}} - l| \quad (1)$$

	0	1	2	3	4	5	6	7	8	9	10	11	...
l (para elétrons)	s	p	d	f	g	h	i	k	l	m	n	o	...

Termos JK para o carbono

$$^2[K]_J$$

$$^2P_{1/2}^{\circ} (J_{\text{caroço}} = 1/2)$$

$$2s^2 2p^1 (^2P_{1/2}^{\circ}) 4f^1$$

$$K = J_{\text{caroço}} + l, J_{\text{caroço}} + l - 1, J_{\text{caroço}} + l - 2, |J_{\text{caroço}} - l| \quad (1)$$

$$K = 1/2 + 3, |1/2 - 3| = 7/2, 5/2$$

	0	1	2	3	4	5	6	7	8	9	10	11	...
l (para elétrons)	s	p	d	f	g	h	i	k	l	m	n	o	...

Termos JK para o carbono

$$^2[K]_J$$

$$2s^2 2p^1 ({}^2P_{1/2}^{\circ}) 4f^1$$

$$^2[7/2]_J \quad ^2[5/2]_J$$

Termos JK para o carbono

$$^2[K]_J$$

$$2s^2 2p^1 ({}^2P_{1/2}^{\circ}) 4f^1$$

$$^2[7/2]_J \quad ^2[5/2]_J$$

Usando a Eq. (2) para calcular os valores de J

$$J = K + s, K + s - 1, K + s - 2, \dots, |K - s| \quad (2)$$

$$s = 1/2$$

Termos JK para o carbono

$$^2[K]_J$$

$$2s^2 2p^1 ({}^2P_{1/2}^{\circ}) 4f^1$$

Para o termo ${}^2[7/2]_J$

$$J = K + s, K + s - 1, K + s - 2 \dots /K - s| \quad (2)$$

$$J = 7/2 + 1/2, 7/2 - 1/2, = 4, 3$$

Termos JK para o carbono

$${}^2[K]_J$$

$$2s^2 2p^1 ({}^2P_{1/2}^{\circ}) 4f^1$$

Obtemos os termos ${}^2[7/2]_{4,3}$

Termos JK para o carbono

$$^2[K]_J$$

$$2s^2 2p^1 ({}^2P_{1/2}^{\circ}) 4f^1$$

Para o termo ${}^2[5/2]_J$

$$J = K + s, K + s - 1, K + s - 2 \dots /K - s| \quad (2)$$

$$s = 1/2$$

$$J = 5/2 + 1/2, 5/2 - 1/2, = 3, 2$$

Termos JK para o carbono

$${}^2[K]_J$$

$$2s^2 2p^1 ({}^2P_{1/2}^{\circ}) 4f^1$$

Obtemos os termos ${}^2[5/2]_{3,2}$

Termos JK para o carbono

$$^2[K]_J$$

$$2s^2 2p^1 ({}^2P_{1/2}^{\circ}) 4f^1$$

Colecionando os termos

$$^2[7/2]_{4,3} \quad ^2[5/2]_{3,2}$$

Termos JK para o carbono

$2s^2 2p({}^2P^{\circ}_{1/2})4f$	${}^2[5/2]$	3	7	83 919.66322
		2	5	83 919.77375
$2s^2 2p({}^2P^{\circ}_{1/2})4f$	${}^2[7/2]$	3	7	83 926.22434
		4	9	83 926.42382
$2s^2 2p4d$	${}^1F^{\circ}$	3	7	83 947.2231
$2s^2 2p({}^2P^{\circ}_{3/2})4f$	${}^2[7/2]$	3	7	83 986.22212
		4	9	83 986.4926
$2s^2 2p({}^2P^{\circ}_{3/2})4f$	${}^2[5/2]$	3	7	84 013.27526
		2	5	84 013.4311
$2s^2 2p({}^2P^{\circ}_{3/2})4f$	${}^2[9/2]$	5	11	84 015.87795
		4	9	84 016.2748
$2s^2 2p4d$	${}^1P^{\circ}$	1	3	84 032.1471
$2s^2 2p({}^2P^{\circ}_{3/2})4f$	${}^2[3/2]$	1	3	84 036.3320
		2	5	84 036.4454

Termos JK para o carbono

$${}^2[K]_J$$

Configuração eletrônica: $2s^2 2p^1 4f^1$

Termos da configuração do caroço $2s^2 2p^1$: ${}^2P_{3/2,1/2}^\circ$

Escolhendo o termo ${}^2P_{3/2}^\circ$ ($J_{\text{caroço}} = 3/2$)

$$2s^2 2p^1 ({}^2P_{3/2}^\circ) 4f^1$$

$$K = J_{\text{caroço}} + l, J_{\text{caroço}} + l - 1, J_{\text{caroço}} + l - 2, \dots, |J_{\text{caroço}} - l| \quad (1)$$

	0	1	2	3	4	5	6	7	8	9	10	11	...
l (para elétrons)	s	p	d	f	g	h	i	k	l	m	n	o	...

Termos JK para o carbono

$$^2[K]_J$$

$$^2P_{3/2}^{\circ} (J_{\text{caroço}} = 3/2)$$

$$2s^2 2p^1 (^2P_{3/2}^{\circ}) 4f^1$$

$$K = J_{\text{caroço}} + l, J_{\text{caroço}} + l - 1, J_{\text{caroço}} + l - 2, \dots, |J_{\text{caroço}} - l| \quad (1)$$

$$K = 3/2 + 3, \dots, |3/2 - 3| = 9/2, 7/2, 5/2, 3/2$$

	0	1	2	3	4	5	6	7	8	9	10	11	...
l (para elétrons)	s	p	d	f	g	h	i	k	l	m	n	o	...

Termos JK para o carbono

$$^2[K]_J$$

$$2s^2 2p^1 ({}^2P_{3/2}^{\circ}) 4f^1$$

$$^2[9/2]_J \quad ^2[7/2]_J \quad ^2[5/2]_J \quad ^2[3/2]_J$$

Termos JK para o carbono

$$^2[K]_J$$

$$2s^2 2p^1 ({}^2P_{1/2}^{\circ}) 4f^1$$

$${}^2[9/2]_J \quad {}^2[7/2]_J \quad {}^2[5/2]_J \quad {}^2[3/2]_J$$

Calculando os valores de J pela eq. (2).

$$J = K + s, K + s - 1, K + s - 2 \dots /K - s| \quad (2)$$

$$s = 1/2$$

Termos JK para o carbono

$$^2[K]_J$$

$$2s^2 2p^1 ({}^2P_{1/2}^{\circ}) 4f^1$$

Para o termo ${}^2[9/2]_J$

$$J = K + s, K + s - 1, K + s - 2 \dots /K - s| \quad (2)$$

$$J = 9/2 + 1/2, 9/2 - 1/2, = 5, 4$$

Termos JK para o carbono

$${}^2[K]_J$$

$$2s^2 2p^1 ({}^2P_{3/2}^{\circ}) 4f^1$$

$$\text{Termos resultantes } {}^2[9/2]_{5,4}$$

Termos JK para o carbono

$$^2[K]_J$$

$$2s^2 2p^1 ({}^2P_{3/2}^{\circ}) 4f^1$$

Para o termo ${}^2[7/2]_J$

$$J = K + s, K + s - 1, K + s - 2 \dots /K - s| \quad (2)$$

$$J = 7/2 + 1/2, 7/2 - 1/2, = 4, 3$$

Termos JK para o carbono

$$^2[K]_J$$

$$2s^2 2p^1 ({}^2P_{3/2}^{\circ}) 4f^1$$

$$\text{Termo resultante } ^2[7/2]_{4,3}$$

Termos JK para o carbono

$${}^2[K]_J$$

$$2s^2 2p^1 ({}^2P_{3/2}^{\circ}) 4f^1$$

Seguindo-se o mesmo procedimento, obtemos

$${}^2[9/2]_{5,4} \quad {}^2[7/2]_{4,3} \quad {}^2[5/2]_{3,2} \quad {}^2[3/2]_{2,1}$$

Termos JK para o carbono

$2s^2 2p({}^2P^{\circ}_{1/2}) 4f$	${}^2[5/2]$	3	7	83 919.66322
		2	5	83 919.77375
$2s^2 2p({}^2P^{\circ}_{1/2}) 4f$	${}^2[7/2]$	3	7	83 926.22434
		4	9	83 926.42382
$2s^2 2p 4d$	${}^1F^{\circ}$	3	7	83 947.2231
$2s^2 2p({}^2P^{\circ}_{3/2}) 4f$	${}^2[7/2]$	3	7	83 986.22212
		4	9	83 986.4926
$2s^2 2p({}^2P^{\circ}_{3/2}) 4f$	${}^2[5/2]$	3	7	84 013.27526
		2	5	84 013.4311
$2s^2 2p({}^2P^{\circ}_{3/2}) 4f$	${}^2[9/2]$	5	11	84 015.87795
		4	9	84 016.2748
$2s^2 2p 4d$	${}^1P^{\circ}$	1	3	84 032.1471
$2s^2 2p({}^2P^{\circ}_{3/2}) 4f$	${}^2[3/2]$	1	3	84 036.3320
		2	5	84 036.4454

Termos JK para o carbono

*Níveis de energia do carbono na configuração eletrônica $2s^2 2p^1 4f^1$

*Kramida, A.; Ralchenko, Yu.; Reader, J.; NIST ASD Team (2021) acessado em 15/10/2022

FIM