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

Roberto B. Faria
faria@iq.ufrj.br
www.iq.ufrj.br/~faria
Instituto de Química
Universidade Federal do Rio de Janeiro

JK coupling

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

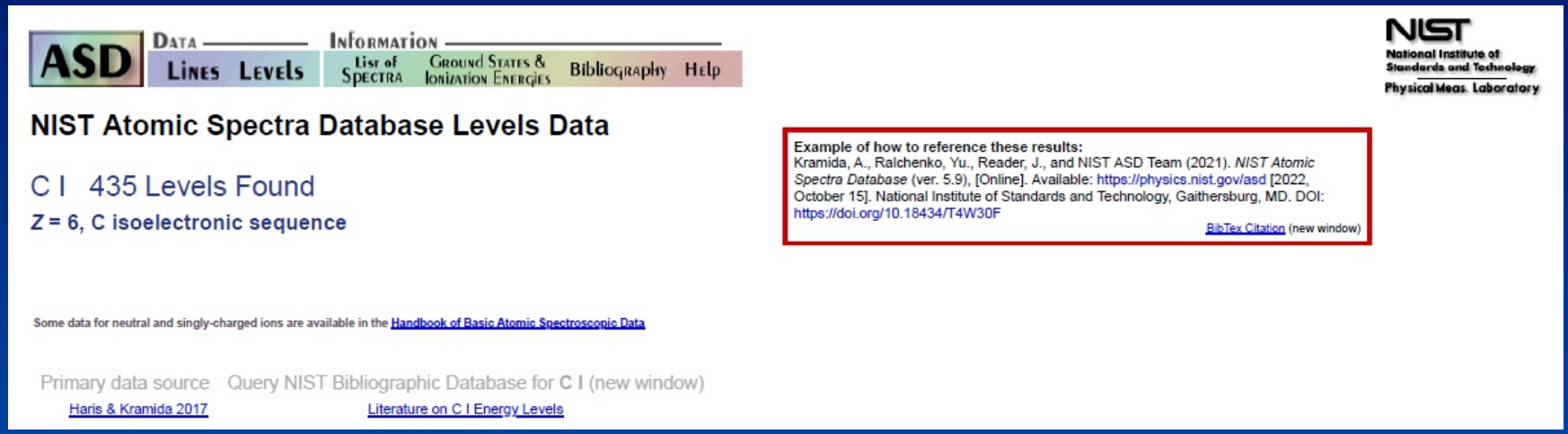
Last update, September 23th, 2024

References

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

JK coupling

JK terms for carbon



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

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: Haris & Kramida 2017

Query NIST Bibliographic Database for **C I** (new window): Literature on C I Energy Levels

JK terms for carbon

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*

JK terms for carbon

$2s^2 2p(^2P^\circ_{1/2})4f$	$^2[^5/_2]$	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

LS coupling

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

LS coupling

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

JK terms for carbon

- Excited states involving one electron in orbitals f or g
- The core electrons interact by *LS* coupling
- The interaction with the excited electron is spin-independent.
- The *JK* scheme consider a new quantum number *K*.
- The *J* value is calculated by eq. (2), where ***s*** is the spin of the electron in the orbital f or g (***s*** = ½)

$$K = J_{\text{core}} + \boldsymbol{\ell} \qquad (1)$$

$$J = K + \boldsymbol{s} \qquad (2)$$

JK terms for carbon

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

The spin multiplicity consider only the spin of the electron in the orbital f or g

$$2S+1 = 2(½) + 1 = 2$$

As a result, all terms are dublets

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

JK terms for carbon

$$^{2}[\mathrm{K}]_{J}$$

Electronic configuration: $2s^2\ 2p^1\ 4f^1$
Core configuration $2s^2\ 2p^1$ terms: $^{2}P_{3/2,1/2}^{\circ}$
Let us choose the term $^{2}P_{1/2}^{\circ}$ ($J_{\mathrm{core}} = ½$)

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

$$K = J_{\mathrm{core}} + \ell,\ J_{\mathrm{core}} + \ell - 1,\ J_{\mathrm{core}} + \ell - 2,\ |J_{\mathrm{core}} - \ell| \qquad (1)$$

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

JK terms for carbon

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

$$^2\mathrm{P}_{1/2}^{\circ}\ (J_{\mathrm{core}} = ½)$$

$$2s^2\ 2p^1\ (^2\mathrm{P}_{1/2}^{\circ})\ 4f^1$$

$$K = J_{\mathrm{core}} + \ell,\ J_{\mathrm{core}} + \ell - 1,\ J_{\mathrm{core}} + \ell - 2,\ |J_{\mathrm{core}} - \ell| \qquad (1)$$

$$K = ½ + 3,\ |½ - 3| = 7/2,\ 5/2$$

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

JK terms for carbon

$$^{2}[\mathrm{K}]_{J}$$

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

$$^{2}[7/2]_{J} \qquad ^{2}[5/2]_{J}$$

JK terms for carbon

$$^{2}[\mathrm{K}]_{J}$$

$$2s^2\ 2p^1\ (^2P_{1/2}°)\ 4f^1$$

$$^{2}[7/2]_{J} \qquad ^{2}[5/2]_{J}$$

Using eq. (2) to calculate the *J* values.

$$J = K + \boldsymbol{s},\ K + \boldsymbol{s} - 1,\ K + \boldsymbol{s} - 2 \ldots |K - \boldsymbol{s}| \qquad (2)$$

$$\boldsymbol{s} = ½$$

JK terms for carbon

$$^{2}[\mathrm{K}]_{J}$$

$$2s^2\ 2p^1\ (^2P_{1/2}°)\ 4f^1$$

For the term $^{2}[7/2]_{J}$

$$J = K + \boldsymbol{s},\ K + \boldsymbol{s} - 1,\ K + \boldsymbol{s} - 2 \ldots |K - \boldsymbol{s}| \qquad (2)$$

$$J = 7/2 + ½,\ 7/2 - ½, = 4, 3$$

JK terms for carbon

$$^{2}[\mathrm{K}]_{J}$$

$2s^2\ 2p^1\ (^2P_{1/2}°)\ 4f^1$

Resulting in terms $^{2}[7/2]_{4,3}$

JK terms for carbon

$$^{2}[\mathrm{K}]_{J}$$

$$2s^2\ 2p^1\ (^2P_{1/2}°)\ 4f^1$$

For the term $^{2}[5/2]_{J}$

$$J = K + \boldsymbol{s},\ K + \boldsymbol{s}\ \text{-}1,\ K + \boldsymbol{s}\ \text{-}\ 2\ \ldots\ |K\ \text{-}\ \boldsymbol{s}| \quad (2)$$

$$\boldsymbol{s} = ½$$

$$J = 5/2 + ½,\ 5/2 - ½,\ = 3,\ 2$$

JK terms for carbon

$$^{2}[\mathrm{K}]_{J}$$

$2s^2\ 2p^1\ (^2P_{1/2}°)\ 4f^1$

Resulting in terms $^{2}[5/2]_{3,2}$

JK terms for carbon

$$^{2}[\mathrm{K}]_{J}$$

$2s^2\ 2p^1\ (^2P_{1/2}°)\ 4f^1$

Colecting the terms

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

JK terms for carbon

$2s^2\ 2p^1\ (^2P_{1/2}°)\ 4f^1$

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

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

$2s^22p(^2P°_{1/2})4f$	$^2[^5/_2]$	3	7	83 919.66322
		2	5	83 919.77375
$2s^22p(^2P°_{1/2})4f$	$^2[^7/_2]$	3	7	83 926.22434
		4	9	83 926.42382
$2s^22p4d$	$^1F°$	3	7	*83 947.2231*
$2s^22p(^2P°_{3/2})4f$	$^2[^7/_2]$	3	7	83 986.22212
		4	9	83 986.4926
$2s^22p(^2P°_{3/2})4f$	$^2[^5/_2]$	3	7	84 013.27526
		2	5	84 013.4311
$2s^22p(^2P°_{3/2})4f$	$^2[^9/_2]$	5	11	84 015.87795
		4	9	84 016.2748
$2s^22p4d$	$^1P°$	1	3	*84 032.1471*
$2s^22p(^2P°_{3/2})4f$	$^2[^3/_2]$	1	3	84 036.3320
		2	5	84 036.4454

JK terms for carbon

$$^{2}[\mathrm{K}]_{J}$$

Electronic configuration: $2s^2\ 2p^1\ 4f^1$
Core configuration $2s^2\ 2p^1$ terms: $^{2}P_{3/2,1/2}^{\circ}$
Let us choose the term $^{2}P_{3/2}^{\circ}$ ($J_{\mathrm{core}} = 3/2$)

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

$$K = J_{\mathrm{core}} + \ell,\ J_{\mathrm{core}} + \ell - 1,\ J_{\mathrm{core}} + \ell - 2,\ |J_{\mathrm{core}} - \ell| \quad (1)$$

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

JK terms for carbon

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

$$^2\mathrm{P}_{3/2}^{\circ}\ (J_{\mathrm{core}} = 3/2)$$

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

$$K = J_{\mathrm{core}} + \ell,\ J_{\mathrm{core}} + \ell - 1,\ J_{\mathrm{core}} + \ell - 2,\ |J_{\mathrm{core}} - \ell| \quad (1)$$

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

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

JK terms for carbon

$$^{2}[\mathrm{K}]_{J}$$

$$2s^2\ 2p^1\ (^2P_{3/2}°)\ 4f^1$$

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

JK terms for carbon

$$^{2}[\mathrm{K}]_{J}$$

$$2s^2\ 2p^1\ (^2P_{1/2}°)\ 4f^1$$

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

$$J = K + \boldsymbol{s},\ K + \boldsymbol{s} - 1,\ K + \boldsymbol{s} - 2 \ \ldots\ |K - \boldsymbol{s}| \qquad (2)$$

$$\boldsymbol{s} = ½$$

JK terms for carbon

$$^{2}[\mathrm{K}]_{J}$$

$$2s^2\ 2p^1\ (^2P_{1/2}°)\ 4f^1$$

For the term $^{2}[9/2]_{J}$

$$J = K + \boldsymbol{s},\ K + \boldsymbol{s} - 1,\ K + \boldsymbol{s} - 2 \ldots |K - \boldsymbol{s}| \qquad (2)$$

$$\boldsymbol{s} = ½$$

$$J = 9/2 + ½,\ 9/2 - ½, = 5, 4$$

JK terms for carbon

$$^{2}[\mathrm{K}]_{J}$$

$2s^2\ 2p^1\ (^2P_{3/2}°)\ 4f^1$

Resulting in terms $^{2}[9/2]_{5,4}$

JK terms for carbon

$$^{2}[\mathrm{K}]_{J}$$

$$2s^2\ 2p^1\ (^2P_{3/2}°)\ 4f^1$$

For the term $^{2}[7/2]_{J}$

$$J = K + \boldsymbol{s},\ K + \boldsymbol{s} - 1,\ K + \boldsymbol{s} - 2 \ldots |K - \boldsymbol{s}| \quad (2)$$

$$\boldsymbol{s} = ½$$

$$J = 7/2 + ½,\ 7/2 - ½, = 4, 3$$

JK terms for carbon

$$^{2}[\mathrm{K}]_{J}$$

$2s^2\ 2p^1\ (^2P_{3/2}°)\ 4f^1$

Resulting in terms $^{2}[7/2]_{4,3}$

JK terms for carbon

$$^{2}[\mathrm{K}]_{J}$$

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

Using a similar procedure

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

JK terms for carbon

$2s^2\ 2p^1\ (^2P_{3/2}°)\ 4f^1$

$^2[9/2]_{5,4}$

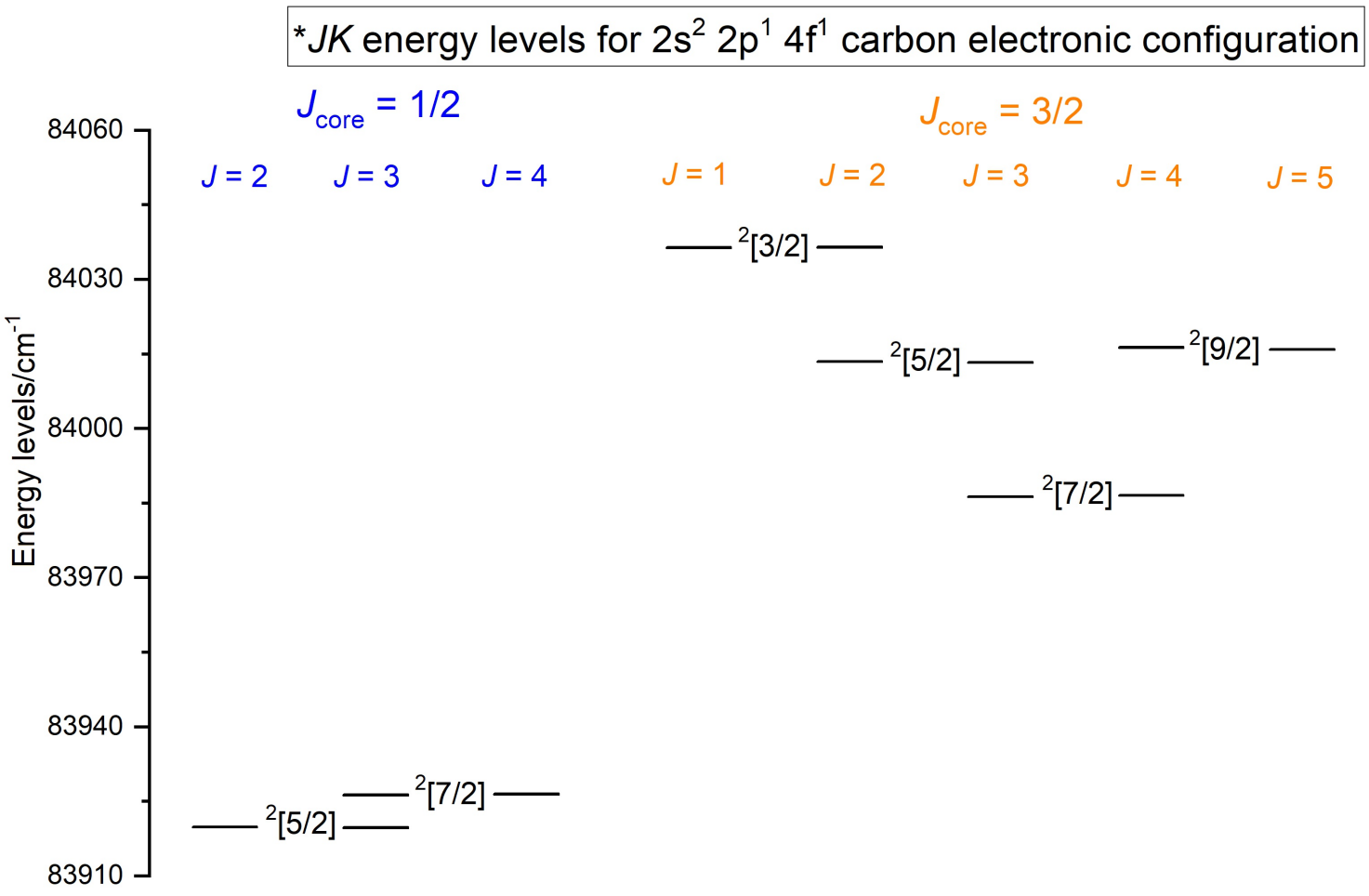
$^2[7/2]_{4,3}$

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

$^2[3/2]_{2,1}$

$2s^22p(^2P°_{1/2})4f$	$^2[^5/_2]$	3	7	83 919.66322
		2	5	83 919.77375
$2s^22p(^2P°_{1/2})4f$	$^2[^7/_2]$	3	7	83 926.22434
		4	9	83 926.42382
$2s^22p4d$	$^1F°$	3	7	*83 947.2231*
$2s^22p(^2P°_{3/2})4f$	$^2[^7/_2]$	3	7	83 986.22212
		4	9	83 986.4926
$2s^22p(^2P°_{3/2})4f$	$^2[^5/_2]$	3	7	84 013.27526
		2	5	84 013.4311
$2s^22p(^2P°_{3/2})4f$	$^2[^9/_2]$	5	11	84 015.87795
		4	9	84 016.2748
$2s^22p4d$	$^1P°$	1	3	*84 032.1471*
$2s^22p(^2P°_{3/2})4f$	$^2[^3/_2]$	1	3	84 036.3320
		2	5	84 036.4454

JK terms for carbon



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

THE END