

Métodos de RMN no estado sólido

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Sumário

■ Fundamentos de RMN:

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 - Spin nuclear.
 - Momento de dipolo magnético.
 - Modelo de camadas.
 - Tabelas de nuclídeos.
 - Momento de quadrupolo elétrico.

Alguns marcos históricos da RMN

- **Rabi (1937):** ressonância em feixes de moléculas de H_2 .
 - Prêmio Nobel de Física - 1944.
- **Bloch (1946):** absorção de RF em água.
 - Prêmio Nobel de Física - 1952.
- **Purcell (1946):** absorção de RF em parafina.
 - Prêmio Nobel de Física - 1952.
- **Hahn (1949):** ecos de spin.
- **Packard (1951):** deslocamento químico em etanol.
- **Andrew, Lowe (1959):** RMN no estado sólido.
- **Ernst (1964):** RMN com transformada de Fourier.
 - Prêmio Nobel de Química - 1991.
- **Wüthrich (1968):** RMN aplicada ao estudo de macromoléculas biológicas.
 - Prêmio Nobel de Química - 2002.
- **Lauterbur, Mansfeld (1973):** imagem por RMN (MRI).
 - Prêmio Nobel de Medicina - 2003.

Spin nuclear e momento de dipolo magnético nuclear

$$\vec{I} = \sum_{k=1}^A (\vec{l}_k + \vec{s}_k)$$

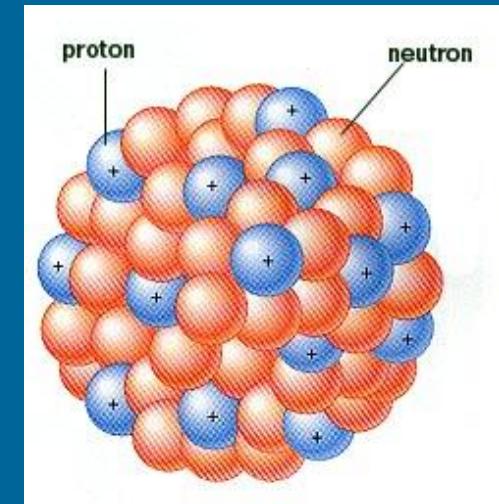
O *spin nuclear*:

- Número quântico *I*.
- Inteiro ou semi-inteiro.

$$\vec{\mu} = (\mu_N / \hbar) \left[\sum_{k=1}^Z \vec{l}_k + \sum_{k=1}^Z g_{sp} \vec{s}_k + \sum_{k=Z+1}^A g_{sn} \vec{s}_k \right]$$

$$g_{sp} = 5,586$$

$$g_{sn} = -3,826$$



Magnéton nuclear:

$$\mu_N = \frac{e\hbar}{2m_p} = 5,051 \times 10^{-27} J / T$$

Magnéton de Bohr:

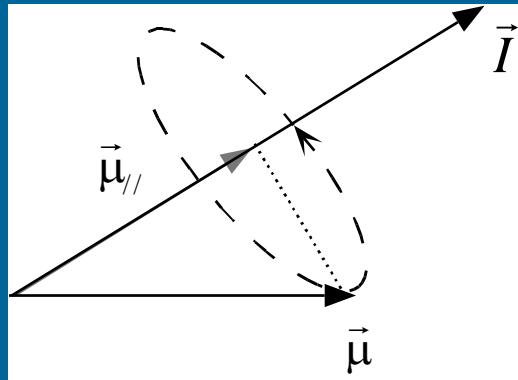
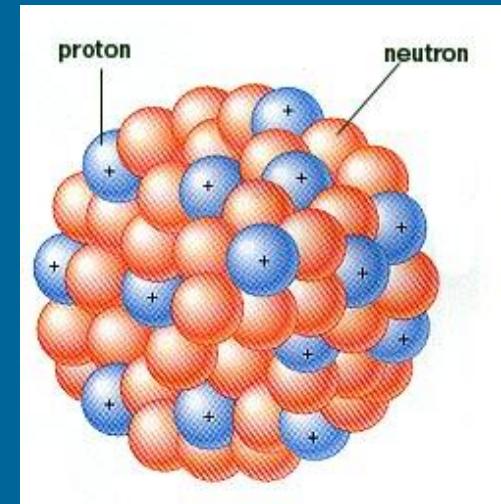
$$\mu_B = \frac{e\hbar}{2m_e} = 9,274 \times 10^{-24} J / T$$

$$g_{se} = -2,002$$

Spin nuclear e momento de dipolo magnético nuclear

$$\vec{I} = \sum_{k=1}^A (\vec{l}_k + \vec{s}_k)$$

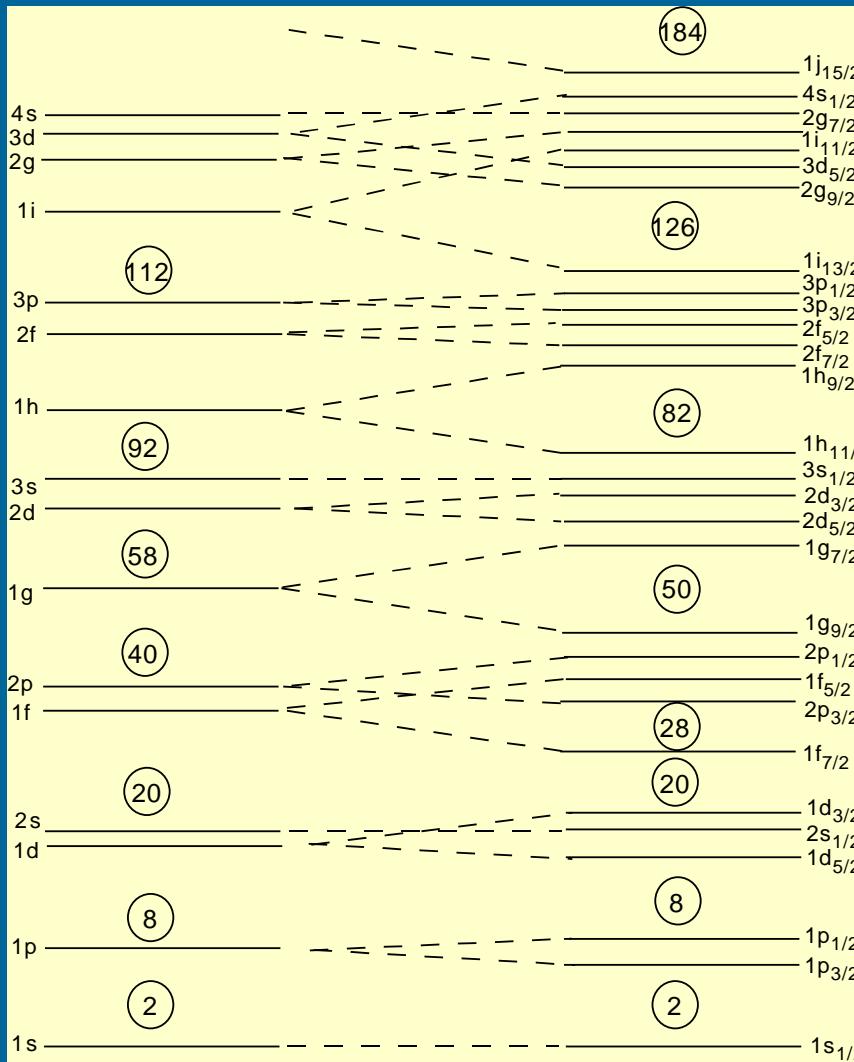
$$\vec{\mu} = (\mu_N / \hbar) \left[\sum_{k=1}^Z \vec{l}_k + \sum_{k=1}^Z g_{sp} \vec{s}_k + \sum_{k=Z+1}^A g_{sn} \vec{s}_k \right]$$



$$\vec{\mu}_{efetivo} = \frac{\langle \vec{\mu} \cdot \vec{I} \rangle}{I(I+1)\hbar^2} \vec{I} = \gamma \vec{I}$$

Fator giromagnético

Modelo de camadas e spin nuclear



Momento angular de cada núcleon:

$$\vec{j} = \vec{l} + \vec{s}$$

$$\mathbf{j} = \mathbf{l} \pm 1/2$$

Notação:

$$n \ l_j$$

Capacidade de cada nível:

$$2j + 1$$

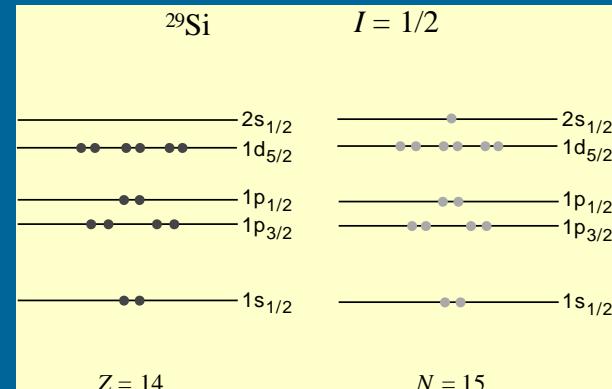
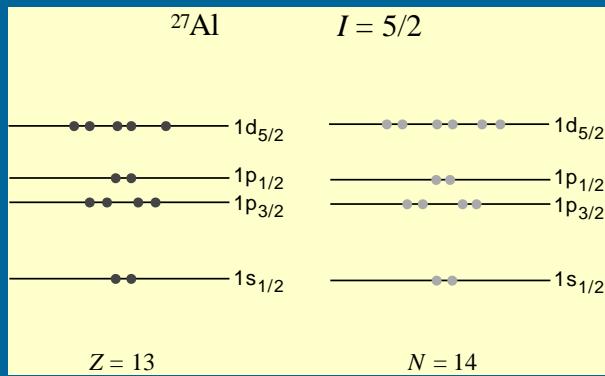
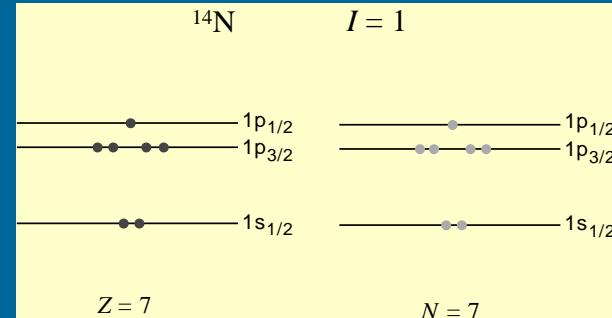
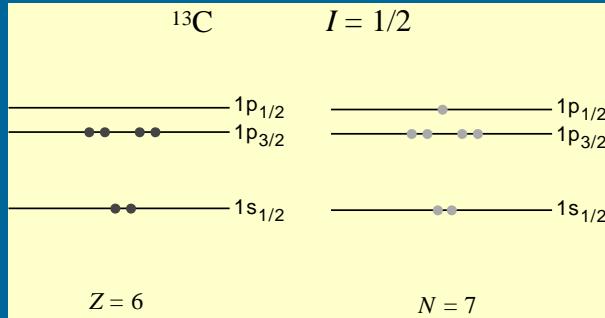
Os núcleos atômicos e a RMN, Freitas & Bonagamba, 1999.

Modelo de camadas e spin nuclear

Previsões do modelo de camadas:

Z	N	A	I	
par	par	par	zero	
par	ímpar	ímpar	semi-inteiro	$I = j_n$
ímpar	par	ímpar	semi-inteiro	$I = j_p$
ímpar	ímpar	par	inteiro	$ j_n - j_p \leq I \leq j_n + j_p$

Modelo de camadas e spin nuclear



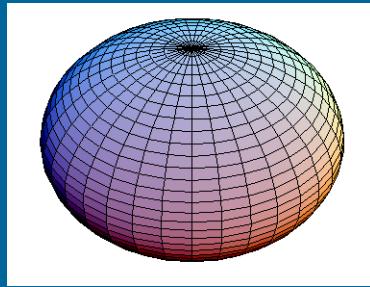
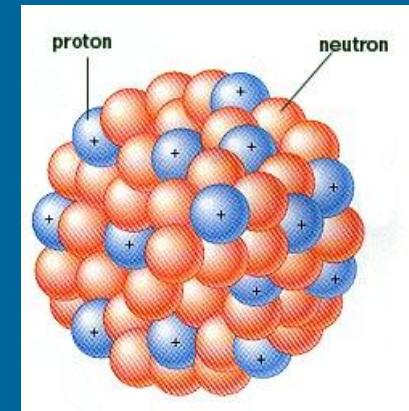
Momento de quadrupolo elétrico nuclear

$$Q_{\alpha\beta} = e \sum_{k=1}^Z (3x_{\alpha k} x_{\beta k} - \delta_{\alpha\beta} r_k^2)$$

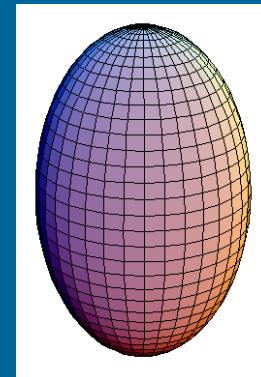
$$Q_{\alpha\beta} = \frac{eQ}{I(2I-1)\hbar^2} \left[\frac{3}{2} \left(\mathbf{I}_\alpha \mathbf{I}_\beta + \mathbf{I}_\beta \mathbf{I}_\alpha \right) - \delta_{\alpha\beta} \mathbf{I}^2 \right]$$

$$eQ = \int (3z'^2 - r'^2) \rho(\vec{r}') d^3 r'$$

$$I > 1/2 \Rightarrow Q \neq 0$$



$Q < 0$ (oblata)



$Q > 0$ (prolata)

Alguns núcleos de interesse para RMN

<i>Nuclídeo</i>	<i>Abundância Natural</i> (%)	<i>I</i>	μ (múltiplos de μ_N)	<i>Q</i> (barns)
1H	99,99	1/2	2,7928	0
^{13}C	1,11	1/2	0,7024	0
^{14}N	99,63	1	0,4036	0,01
^{15}N	0,37	1/2	0,2831	0
^{19}F	100	1/2	2,6287	0
^{27}Al	100	5/2	3,6414	0,150
^{29}Si	4,70	1/2	0,5553	0
^{31}P	100	1/2	1,1317	0
^{55}Mn	100	5/2	3,4680	0,400
^{59}Co	100	7/2	4,6490	0,400
^{155}Gd	14,73	3/2	0,2700	1,300
^{157}Gd	15,68	3/2	0,3600	1,500

Propriedades de alguns núcleos de interesse para RMN

TABLE 1
The Spin Properties of Spin-1/2 Nuclei

Isotope	Natural abundance (x/%)	Magnetic moment (μ/μ_N)	Magnetogyric ratio ($\gamma/10^7 \text{ rad s}^{-1} \text{ T}^{-1}$)	Frequency ratio ($\mathcal{E}/\%$)	Reference compound	Sample conditions	Relative receptivity	
							D^p	D^c
¹ H	99.9885	4.837 353 570	26.752 2128	100.000 000	Me ₄ Si	CDCl ₃ , $\varphi = 1\%$	1.000	5.87×10^3
³ H	—	5.159 714 367	28.534 9779	106.663 974	Me ₄ Si- <i>t</i> ₁	See lit.	—	—
³ He	1.37×10^{-4}	-3.685 154 336	-20.380 1587	76.179 437	He	Gas	6.06×10^{-7}	3.56×10^{-3}
¹³ C	1.07	1.216 613	6.728 284	25.145 020	Me ₄ Si	CDCl ₃ , $\varphi = 1\%$	1.70×10^{-4}	1.00
¹⁵ N	0.368	-0.490 497 46	-2.712 618 04	10.136 767	MeNO ₂	Neat/CDCl ₃	3.84×10^{-6}	2.25×10^{-2}
¹⁹ F	100	4.553 333	25.181 48	94.094 011	CCl ₃ F	See lit.	0.834	4.90×10^3
²⁹ Si	4.6832	-0.961 79	-5.3190	19.867 187	Me ₄ Si	CDCl ₃ , $\varphi = 1\%$	3.68×10^{-4}	2.16
³¹ P	100	1.959 99	10.8394	40.480 742	H ₃ PO ₄	See lit.	6.65×10^{-2}	3.91×10^2
⁵⁷ Fe	2.119	0.156 9636	0.868 0624	3.237 778	Fe(CO) ₅	C ₆ D ₆	7.24×10^{-7}	4.25×10^{-3}
⁷⁷ Se	7.63	0.926 775 77	5.125 3857	19.071 513	Me ₂ Se	Neat/C ₆ D ₆	5.37×10^{-4}	3.15
⁸⁹ Y	100	-0.238 010 49	-1.316 2791	4.900 198	Y(NO ₃) ₃	H ₂ O/D ₂ O	1.19×10^{-4}	0.700
¹⁰³ Rh	100	-0.1531	-0.8468	3.186 447	Rh(acac) ₃	CDCl ₃ , sat.	3.17×10^{-5}	0.186
(¹⁰⁷ Ag)	51.839	-0.196 898 93	-1.088 9181	4.047 819	AgNO ₃	D ₂ O, sat.	3.50×10^{-5}	0.205
¹⁰⁹ Ag	48.161	-0.226 362 79	-1.251 8634	4.653 533	AgNO ₃	D ₂ O, sat.	4.94×10^{-5}	0.290
(¹¹¹ Cd)	12.80	-1.030 3729	-5.698 3131	21.215 480	Me ₂ Cd	Neat	1.24×10^{-3}	7.27
¹¹³ Cd	12.22	-1.077 8568	-5.960 9155	22.193 175	Me ₂ Cd	Neat	1.35×10^{-3}	7.94
(¹¹⁵ Sn)	0.34	-1.5915	-8.8013	32.718 749	Me ₄ Sn	Neat/C ₆ D ₆	1.21×10^{-4}	0.711
(¹¹⁷ Sn)	7.68	-1.733 85	-9.588 79	35.632 259	Me ₄ Sn	Neat/C ₆ D ₆	3.54×10^{-3}	20.8
¹¹⁹ Sn	8.59	-1.813 94	-10.0317	37.290 632	Me ₄ Sn	Neat/C ₆ D ₆	4.53×10^{-3}	26.6
(¹²³ Te)	0.89	-1.276 431	-7.059 098	26.169 742	Me ₂ Te	Neat/C ₆ D ₆	1.64×10^{-4}	0.961
¹²⁵ Te	7.07	-1.538 9360	-8.510 8404	31.549 769	Me ₂ Te	Neat/C ₆ D ₆	2.28×10^{-3}	13.4
¹²⁹ Xe	26.44	-1.347 494	-7.452 103	27.810 186	XeOF ₄	Neat	5.72×10^{-3}	33.6
¹⁸³ W	14.31	0.204 009 19	1.128 2403	4.166 387	Na ₂ WO ₄	D ₂ O, 1 M	1.07×10^{-5}	6.31×10^{-2}
¹⁸⁷ Os	1.96	0.111 9804	0.619 2895	2.282 331	OsO ₄	CCl ₄ , 0.98 M	2.43×10^{-7}	1.43×10^{-3}
¹⁹⁵ Pt	33.832	1.0557	5.8385	21.496 784	Na ₂ PtCl ₆	D ₂ O, 1.2 M	3.51×10^{-3}	20.7
¹⁹⁹ Hg	16.87	0.876 219 37	4.845 7916	17.910 822	Me ₂ Hg ^a	Neat	1.00×10^{-3}	5.89
(²⁰³ Tl)	29.524	2.809 833 05	15.539 3338	57.123 200	Tl(NO ₃) ₃	See lit.	5.79×10^{-2}	3.40×10^2
²⁰⁵ Tl	70.476	2.837 470 94	15.692 1808	57.683 838	Tl(NO ₃) ₃	See lit.	0.142	8.36×10^2
²⁰⁷ Pb	22.1	1.009 06	5.580 46	20.920 599	Me ₄ Pb	Neat/C ₆ D ₆	2.01×10^{-3}	11.8

Note. Taken from *Pure Appl. Chem.* **73**, 1795 (2001). © IUPAC 2001 Full text at <http://www.iupac.org/publications/pac/2001/7311/7311x1795.html>.

^a Highly toxic. Do not handle directly. Some other reference compounds are toxic. The unified scale should always be used in these cases.

Propriedades de alguns núcleos de interesse para RMN

TABLE 2
The Spin Properties of Quadrupolar Nuclei

Isotope	Spin	Natural abundance (x/%)	Magnetic moment (μ/μ_N)	Magnetogyric ratio ($\gamma/10^7 \text{ rad s}^{-1} \text{ T}^{-1}$)	Quadrupole moment (Q/fm^2)	Frequency ratio ($\mathcal{E}/\%$)	Reference sample	Sample conditions	Line-width factor (ℓ/fm^4)	Relative receptivity	
										D^p	D^C
² H	1	0.0115	1.212 600 77	4.106 627 91	0.2860	15.350 609	(CD ₃) ₄ Si	CDCl ₃ $\varphi = 1\%$	0.41	1.11×10^{-6}	6.52×10^{-3}
⁶ Li	1	7.59	1.162 5637	3.937 1709	-0.0808	14.716 086	LiCl	D ₂ O, 9.7 m	0.033	6.45×10^{-4}	3.79
⁷ Li	3/2	92.41	4.204 075 05	10.397 7013	-4.01	38.863 797	LiCl	D ₂ O, 9.7 m	21	0.271	1.59×10^3
⁹ Be	3/2	100	-1.520 136	-3.759 666	5.288	14.051 813	BeSO ₄	D ₂ O, 0.43 m	37	1.39×10^{-2}	81.5
¹⁰ B	3	19.9	2.079 2055	2.874 6786	8.459	10.743 658	BF ₃ ·Et ₂ O	CDCl ₃	14	3.95×10^{-3}	23.2
¹¹ B	3/2	80.1	3.471 0308	8.584 7044	4.059	32.083 974	BF ₃ ·Et ₂ O	CDCl ₃	22	0.132	7.77×10^2
¹⁴ N	1	99.632	0.571 004 28	1.933 7792	2.044	7.226 317	CH ₃ NO ₂	Neat/CDCl ₃	21	1.00×10^{-3}	5.90
¹⁷ O	5/2	0.038	-2.240 77	-3.628 08	-2.558	13.556 457	D ₂ O	Neat	2.1	1.11×10^{-5}	6.50×10^{-2}
²¹ Ne	3/2	0.27	-0.854 376	-2.113 08	10.155	7.894 296	Ne	Gas, 1.1 MPa	140	6.65×10^{-6}	3.91×10^{-2}
²³ Na	3/2	100	2.862 9811	7.080 8493	10.4	26.451 900	NaCl	D ₂ O, 0.1 M	140	9.27×10^{-2}	5.45×10^2
²⁵ Mg	5/2	10.00	-1.012 20	-1.638 87	19.94	6.121 635	MgCl ₂	D ₂ O, 11 M	130	2.68×10^{-4}	1.58
²⁷ Al	5/2	100	4.308 6865	6.976 2715	14.66	26.056 859	Al(NO ₃) ₃	D ₂ O, 1.1 m	69	0.207	1.22×10^3
³³ S	3/2	0.76	0.831 1696	2.055 685	-6.78	7.676 000	(NH ₄) ₂ SO ₄	D ₂ O, sat.	61	1.72×10^{-5}	0.101
³⁵ Cl	3/2	75.78	1.061 035	2.624 198	-8.165	9.797 909	NaCl	D ₂ O, 0.1 M	89	3.58×10^{-3}	21.0
³⁷ Cl	3/2	24.22	0.883 1998	2.184 368	-6.435	8.155 725	NaCl	D ₂ O, 0.1 M	55	6.59×10^{-4}	3.87
³⁹ K	3/2	93.2581	0.505 433 76	1.250 0608	5.85	4.666 373	KCl	D ₂ O, 0.1 M	46	4.76×10^{-4}	2.79
(⁴⁰ K)	4	0.0117	-1.451 3203	-1.554 2854	-7.3	5.802 018	KCl	D ₂ O, 0.1 M	5.2	6.12×10^{-7}	3.59×10^{-3}
(⁴¹ K)	3/2	6.7302	0.277 396 09	0.686 068 08	7.11	2.561 305	KCl	D ₂ O, 0.1 M	67	5.68×10^{-6}	3.33×10^{-2}
⁴³ Ca	7/2	0.135	-1.494 067	-1.803 069	-4.08	6.730 029	CaCl ₂	D ₂ O, 0.1 M	2.3	8.68×10^{-6}	5.10×10^{-2}
⁴⁵ Sc	7/2	100	5.393 3489	6.508 7973	-22.0	24.291 747	Sc(NO ₃) ₃	D ₂ O, 0.06 M	66	0.302	1.78×10^3
⁴⁷ Ti	5/2	7.44	-0.932 94	-1.510 5	30.2	5.637 534	TiCl ₄	Neat	290	1.56×10^{-4}	0.918
⁴⁹ Ti	7/2	5.41	-1.252 01	-1.510 95	24.7	5.639 037	TiCl ₄	Neat	83	2.05×10^{-4}	1.20
(⁵⁰ V)	6	0.250	3.613 7570	2.670 6490	21.0	9.970 309	VOCl ₃	Neat/C ₆ D ₆	17	1.39×10^{-4}	0.818
⁵¹ V	7/2	99.750	5.838 0835	7.045 5117	-5.2	26.302 948	VOCl ₃	Neat/C ₆ D ₆	3.7	0.383	2.25×10^3
⁵³ Cr	3/2	9.501	-0.612 63	-1.5152	-15.0	5.652 496	K ₂ CrO ₄	D ₂ O, sat.	300	8.63×10^{-5}	0.507
⁵⁵ Mn	5/2	100	4.104 2437	6.645 2546	33.0	24.789 218	KMnO ₄	D ₂ O, 0.82 m	350	0.179	1.05×10^3
⁵⁹ Co	7/2	100	5.247	6.332	42.0	23.727 074	K ₃ [Co(CN) ₆]	D ₂ O, 0.56 m	240	0.278	1.64×10^3
⁶¹ Ni	3/2	1.1399	-0.968 27	-2.3948	16.2	8.936 051	Ni(CO) ₄	Neat/C ₆ D ₆	350	4.09×10^{-5}	0.240
⁶³ Cu	3/2	69.17	2.875 4908	7.111 7890	-22.0	26.515 473	[Cu(CH ₃ CN) ₄][ClO ₄]	CH ₃ CN, sat.	650	6.50×10^{-2}	3.82×10^2
⁶⁵ Cu	3/2	30.83	3.074 65	7.604 35	-20.4	28.403 693	[Cu(CH ₃ CN) ₄][ClO ₄]	CH ₃ CN, sat.	550	3.54×10^{-2}	2.08×10^2
⁶⁷ Zn	5/2	4.10	1.035 556	1.676 688	15.0	6.256 803	Zn(NO ₃) ₂	D ₂ O, sat.	72	1.18×10^{-4}	0.692
(⁶⁹ Ga)	3/2	60.108	2.603 405	6.438 855	17.1	24.001 354	Ga(NO ₃) ₃	D ₂ O, 1.1 m	390	4.19×10^{-2}	2.46×10^2
⁷¹ Ga	3/2	39.892	3.307 871	8.181 171	10.7	30.496 704	Ga(NO ₃) ₃	D ₂ O, 1.1 m	150	5.71×10^{-2}	3.35×10^2
⁷³ Ge	9/2	7.73	-0.972 2881	-0.936 0303	-19.6	3.488 315	(CH ₃) ₄ Ge	Neat	28	1.09×10^{-4}	0.642
⁷⁵ As	3/2	100	1.858 354	4.596 163	31.4	17.122 614	NaAsF ₆	CD ₃ CN, 0.5 M	1300	2.54×10^{-2}	1.49×10^2

R. K. HARRIS *et al.* © 2001 IUPAC, *Pure and Applied Chemistry* 73, 1795–1818

Propriedades de alguns núcleos de interesse para RMN

TABLE 2
The Spin Properties of Quadrupolar Nuclei

Isotope	Spin	Natural abundance (x/%)	Magnetic moment (μ/μ_N)	Magnetogyric ratio ($\gamma/10^7 \text{ rad s}^{-1} \text{ T}^{-1}$)	Quadrupole moment (Q/fm^2)	Frequency ratio ($\mathcal{E}/\%$)	Reference sample	Sample conditions	Line-width factor (ℓ/fm^4)	Relative receptivity	
										D^p	D^c
(⁷⁹ Br)	3/2	50.69	2.719 351	6.725 616	31.3	25.053 980	NaBr	D_2O , 0.01 M	1300	4.03×10^{-2}	2.37×10^2
(⁸¹ Br)	3/2	49.31	2.931 283	7.249 776	26.2	27.006 518	NaBr	D_2O , 0.01 M	920	4.91×10^{-2}	2.88×10^2
(⁸³ Kr)	9/2	11.49	-1.073 11	-1.033 10	25.9	3.847 600	Kr	Gas	50	2.18×10^{-4}	1.28
(⁸⁵ Rb)	5/2	72.17	1.601 3071	2.592 7050	27.6	9.654 943	RbCl	D_2O , 0.01 M	240	7.67×10^{-3}	45.0
(⁸⁷ Rb)	3/2	27.83	3.552 582	8.786 400	13.35	32.720 454	RbCl	D_2O , 0.01 M	240	4.93×10^{-2}	2.90×10^2
(⁸⁷ Sr)	9/2	7.00	-1.209 0236	-1.163 9376	33.5	4.333 822	SrCl_2	D_2O , 0.5 M	83	1.90×10^{-4}	1.12
(⁹¹ Zr)	5/2	11.22	-1.542 46	-2.497 43	-17.6	9.296 298	$(\text{Zr}(\text{C}_5\text{H}_5)_2\text{Cl}_2$	CH_2Cl_2 , sat.	99	1.07×10^{-3}	6.26
(⁹³ Nb)	9/2	100	6.8217	6.5674	-32.0	24.476 170	K[NbCl ₆]	CH_3CN , sat.	76	0.488	2.87×10^3
(⁹⁵ Mo)	5/2	15.92	-1.082	-1.751	-2.2	6.516 926	Na_2MoO_4	D_2O , 2 M	1.5	5.21×10^{-4}	3.06
(⁹⁷ Mo)	5/2	9.55	-1.105	-1.788	25.5	6.653 695	Na_2MoO_4	D_2O , 2 M	210	3.33×10^{-4}	1.95
(⁹⁹ Tc)	9/2	—	6.281	6.046	-12.9	22.508 326	NH_4TcO_4	D_2O	12	—	—
(⁹⁹ Ru)	5/2	12.76	-0.7588	-1.229	7.9	4.605 151	K ₄ [Ru(CN) ₆]	D_2O , 0.3 M	20	1.44×10^{-4}	0.848
(¹⁰¹ Ru)	5/2	17.06	-0.8505	-1.377	45.7	5.161 369	K ₄ [Ru(CN) ₆]	D_2O , 0.3 M	670	2.71×10^{-4}	1.59
(¹⁰⁵ Pd)	5/2	22.33	-0.760	-1.23	66.0	4.576 100	K ₂ PdCl ₆	D_2O , sat.	1400	2.53×10^{-4}	1.49
(¹¹³ In)	9/2	4.29	6.1124	5.8845	79.9	21.865 755	In(NO ₃) ₃	D_2O , 0.1 M	470	1.51×10^{-2}	88.5
(¹¹⁵ In)	9/2	95.71	6.1256	5.8972	81.0	21.912 629	In(NO ₃) ₃	D_2O , 0.1 M	490	0.338	1.98×10^3
(¹²¹ Sb)	5/2	57.21	3.9796	6.4435	-36.0	23.930 577	K ₃ SbCl ₆	CH_3CN , sat.	410	9.33×10^{-2}	5.48×10^2
(¹²³ Sb)	7/2	42.79	2.8912	3.4892	-49.0	12.959 217	K ₃ SbCl ₆	CH_3CN , sat.	330	1.99×10^{-2}	1.17×10^2
(¹²⁷ I)	5/2	100	3.328 710	5.389 573	-71.0	20.007 486	KI	D_2O , 0.01 M	1600	9.54×10^{-2}	5.60×10^2
(¹³¹ Xe)	3/2	21.18	0.893 1899	2.209 076	-11.4	8.243 921	XeOF ₄	Neat	170	5.96×10^{-4}	3.50
(¹³³ Cs)	7/2	100	2.927 7407	3.533 2539	-0.343	13.116 142	CsNO ₃	D_2O , 0.1 M	0.016	4.84×10^{-2}	2.84×10^2
(¹³⁵ Ba)	3/2	6.592	1.081 78	2.675 50	16.0	9.934 457	BaCl ₂	D_2O , 0.5 M	340	3.30×10^{-4}	1.93
(¹³⁷ Ba)	3/2	11.232	1.210 13	2.992 95	24.5	11.112 928	BaCl ₂	D_2O , 0.5 M	800	7.87×10^{-4}	4.62
(¹³⁸ La)	5	0.090	4.068 095	3.557 239	45.0	13.194 300	LaCl ₃	$\text{D}_2\text{O}/\text{H}_2\text{O}$	120	8.46×10^{-5}	0.497
(¹³⁹ La)	7/2	99.910	3.155 6770	3.808 3318	20.0	14.125 641	LaCl ₃	D_2O , 0.01 M	54	6.05×10^{-2}	3.56×10^2
(¹⁷⁷ Hf)	7/2	18.60	0.8997	1.086	336.5	(4.007)	—	—	1.5×10^4	2.61×10^{-4}	1.54
(¹⁷⁹ Hf)	9/2	13.62	-0.7085	-0.6821	379.3	(2.517)	—	—	1.1×10^4	7.45×10^{-5}	0.438
(¹⁸¹ Ta)	7/2	99.988	2.6879	3.2438	317.0	11.989 600	KTaCl ₆	CH_3CN , sat.	1.4×10^4	3.74×10^{-2}	2.20×10^2
(¹⁸⁵ Re)	5/2	37.40	3.7710	6.1057	218.0	22.524 600	KReO ₄	D_2O , 0.1 M	1.5×10^4	5.19×10^{-2}	3.05×10^2
(¹⁸⁷ Re)	5/2	62.60	3.8096	6.1682	207.0	22.751 600	KReO ₄	D_2O , 0.1 M	1.4×10^4	8.95×10^{-2}	5.26×10^2
(¹⁸⁹ Os)	3/2	16.15	0.851 970	2.107 13	85.6	7.765 400	OsO ₄	CCl ₄ , 0.98 M	9800	3.95×10^{-4}	2.32
(¹⁹¹ Ir)	3/2	37.3	0.1946	0.4812	81.6	(1.718)	—	—	8900	1.09×10^{-5}	6.38×10^{-2}
(¹⁹³ Ir)	3/2	62.7	0.2113	0.5227	75.1	(1.871)	—	—	7500	2.34×10^{-5}	0.137
(¹⁹⁷ Au)	3/2	100	0.191 271	0.473 060	54.7	(1.729)	—	—	4000	2.77×10^{-5}	0.162
(²⁰¹ Hg)	3/2	13.18	-0.723 2483	-1.788 769	38.6	6.611 583	(CH ₃) ₂ Hg ⁶	Neat	2000	1.97×10^{-4}	1.16
(²⁰⁹ Bi)	9/2	100	4.5444	4.3750	-51.6	16.069 288	Bi(NO ₃) ₂	HNO ₃ /D ₂ O/H ₂ O	200	0.144	8.48×10^2

Note. Taken from *Pure Appl. Chem.* **73**, 1795 (2001). © IUPAC 2001. Full text at <http://www.iupac.org/publications/pac/7311/7311x1795.html>.

^a Highly toxic. Do not handle directly. Some other reference compounds are toxic. The unified scale should always be used in these cases.

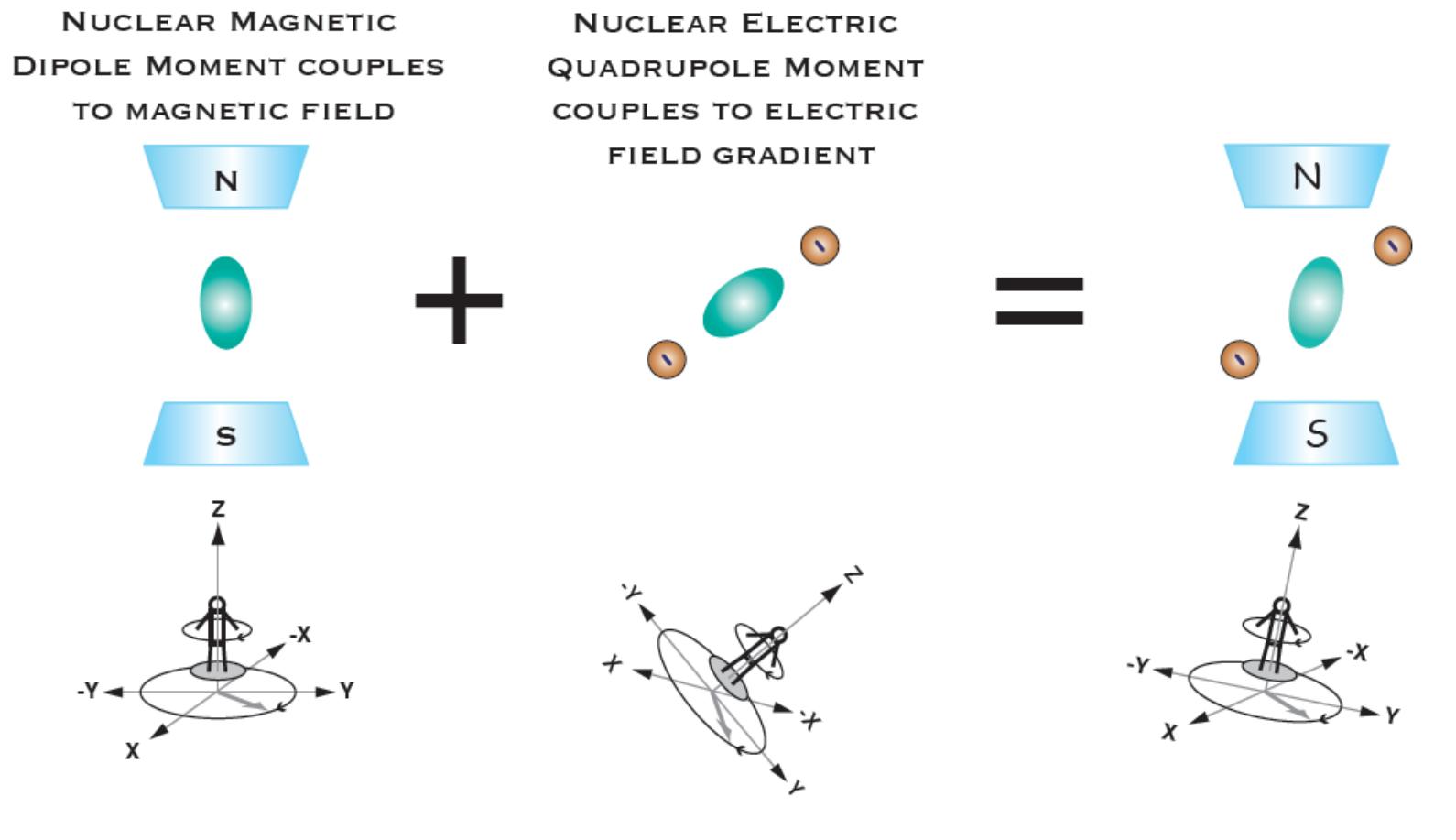
Alguns núcleos de interesse para RMN

MOST ABUNDANT NMR ACTIVE NUCLEI

IA	IIA	Spin = $\frac{1}{2}$												VIIIA				
H	Be	Li	Mg	Na	Al	Si	P	S	Cl	Ar	B	C	N	O	F	He		
Fr	Rd	Ac	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn	
VIIIB																		
IB																		
IIB																		
Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu					
Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr					

<http://www.grandinetti.org/Research/NMR>

Interação nuclear combinada: magnética e elétrica



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