

Métodos de RMN no estado sólido

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- Fundamentos de RMN:
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 - Momento de dipolo magnético.
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 - 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.

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

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

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

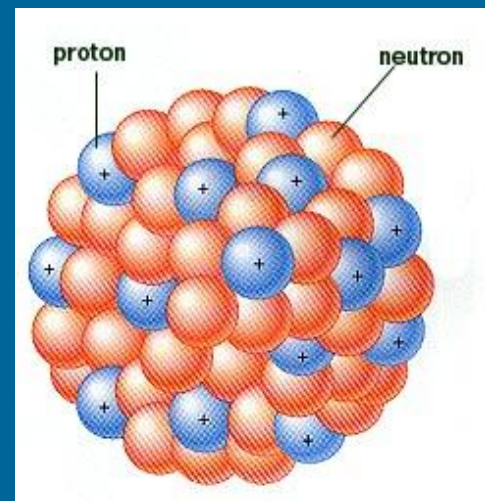
Magnéton nuclear:

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

Magnéton de Bohr:

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

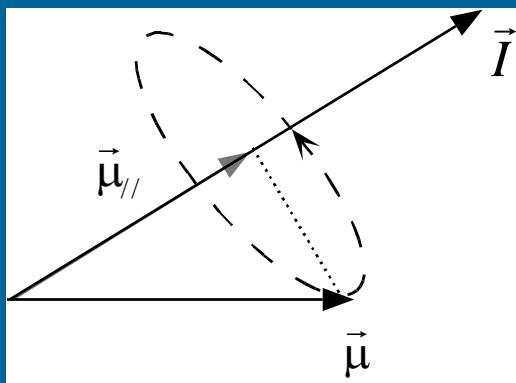
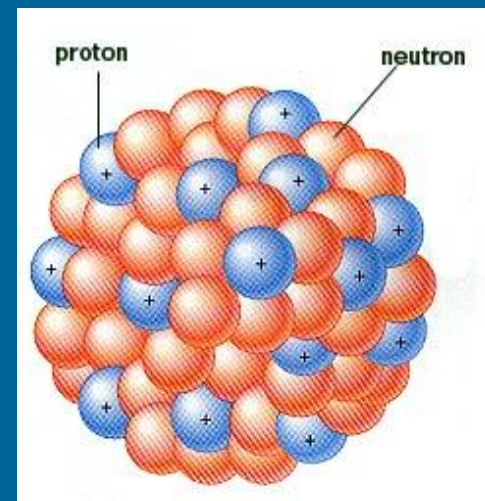
$$g_{se} = -2,002$$



Spin nuclear e momento de dipolo magnético nuclear

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

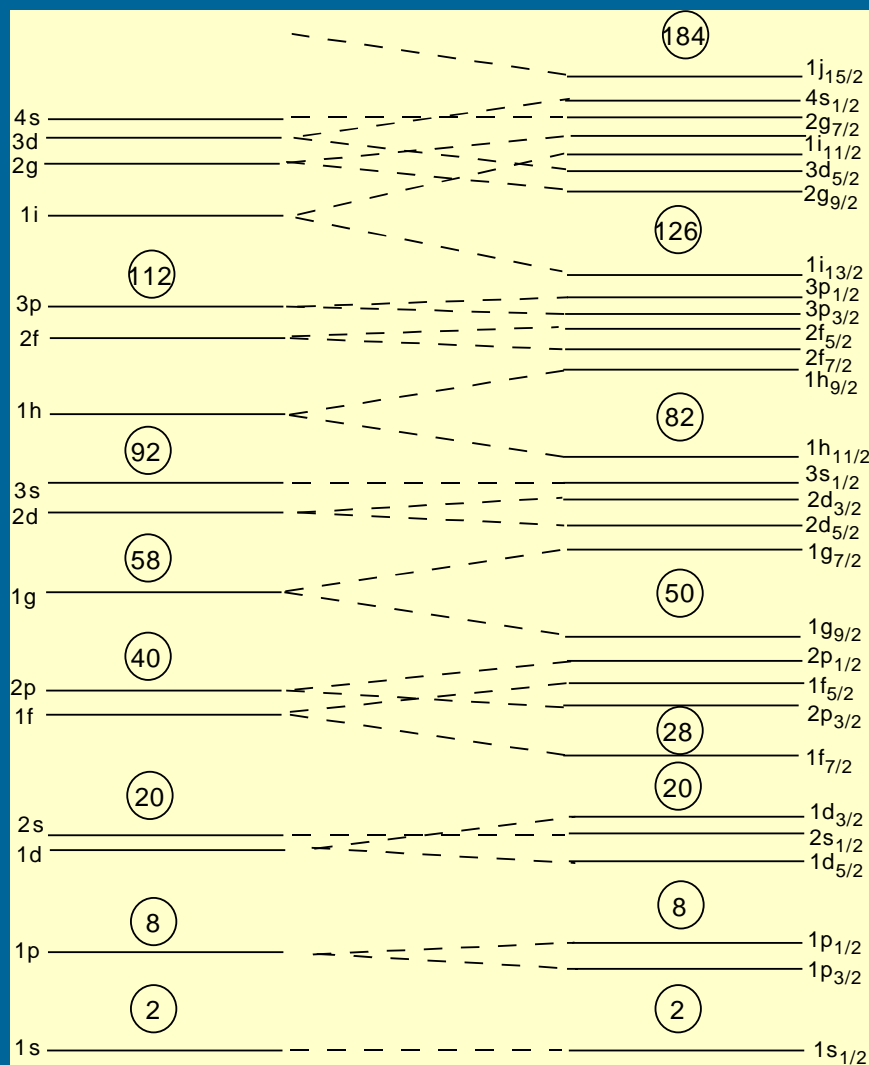
$$\vec{\mu} = (\mu_N / \hbar) \left[\sum_{k=1}^Z \vec{l}_k + \sum_{k=1}^Z g_{sp} \vec{s}_k + \sum_{k=Z+1}^A g_{sn} \vec{s}_k \right]$$



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

Fator giromagnético

Modelo de camadas e spin nuclear



Momento angular de cada núcleon:

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

$$j = l \pm 1/2$$

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:

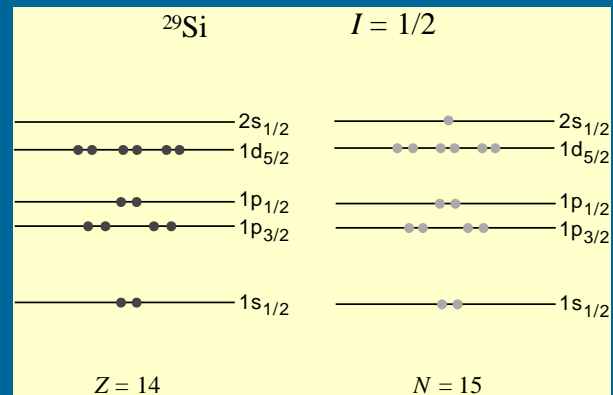
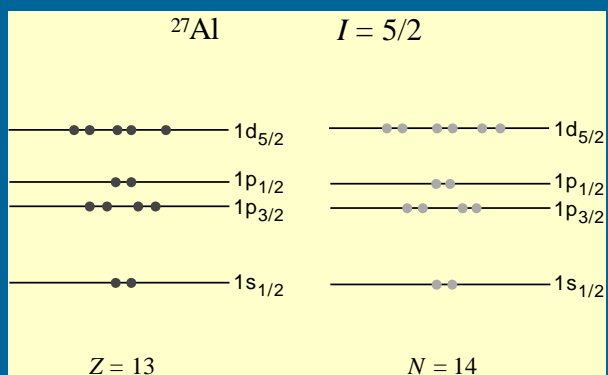
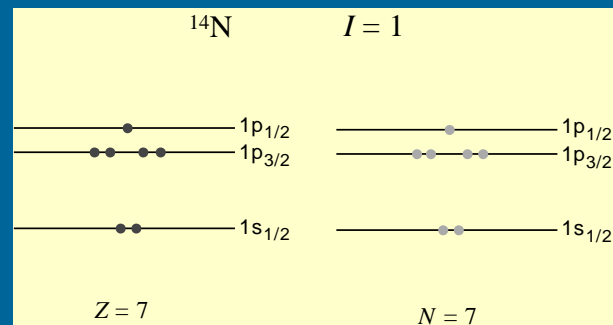
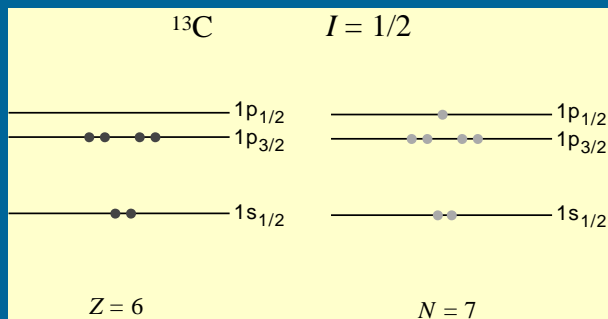
Z	N	A	I
par	par	par	zero
par	ímpar	ímpar	semi-inteiro
ímpar	par	ímpar	semi-inteiro
ímpar	ímpar	par	inteiro

$$I = j_n$$

$$I = j_p$$

$$|j_n - j_p| \leq I \leq j_n + j_p$$

Modelo de camadas e spin nuclear



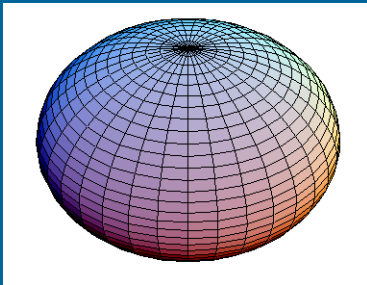
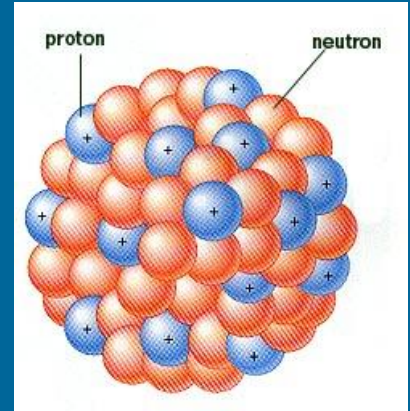
Momento de quadrupolo elétrico nuclear

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

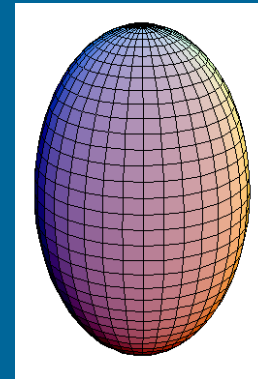
$$Q_{\alpha\beta} = \frac{eQ}{I(2I-1)\hbar^2} \left[\frac{3}{2} (\mathbf{I}_\alpha \mathbf{I}_\beta + \mathbf{I}_\beta \mathbf{I}_\alpha) - \delta_{\alpha\beta} \mathbf{I}^2 \right]$$

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

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



$Q < 0$ (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)	Q (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
^1H	99.9885	4.837 353 570	26.752 2128	100.000 000	Me_4Si	CDCl_3 , $\varphi = 1\%$	1.000	5.87×10^3
^3H	—	5.159 714 367	28.534 9779	106.663 974	$\text{Me}_4\text{Si-}t_1$	See lit.	—	—
^3He	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_4Si	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_3F	See lit.	0.834	4.90×10^3
^{29}Si	4.6832	−0.961 79	−5.3190	19.867 187	Me_4Si	CDCl_3 , $\varphi = 1\%$	3.68×10^{-4}	2.16
^{31}P	100	1.959 99	10.8394	40.480 742	H_3PO_4	See lit.	6.65×10^{-2}	3.91×10^2
^{57}Fe	2.119	0.156 9636	0.868 0624	3.237 778	$\text{Fe}(\text{CO})_5$	C_6D_6	7.24×10^{-7}	4.25×10^{-3}
^{77}Se	7.63	0.926 775 77	5.125 3857	19.071 513	Me_2Se	Neat/ C_6D_6	5.37×10^{-4}	3.15
^{89}Y	100	−0.238 010 49	−1.316 2791	4.900 198	$\text{Y}(\text{NO}_3)_3$	$\text{H}_2\text{O}/\text{D}_2\text{O}$	1.19×10^{-4}	0.700
^{103}Rh	100	−0.1531	−0.8468	3.186 447	$\text{Rh}(\text{acac})_3$	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_2O , sat.	3.50×10^{-5}	0.205
^{109}Ag	48.161	−0.226 362 79	−1.251 8634	4.653 533	AgNO_3	D_2O , sat.	4.94×10^{-5}	0.290
^{111}Cd	12.80	−1.030 3729	−5.698 3131	21.215 480	Me_2Cd	Neat	1.24×10^{-3}	7.27
^{113}Cd	12.22	−1.077 8568	−5.960 9155	22.193 175	Me_2Cd	Neat	1.35×10^{-3}	7.94
^{115}Sn	0.34	−1.5915	−8.8013	32.718 749	Me_4Sn	Neat/ C_6D_6	1.21×10^{-4}	0.711
^{117}Sn	7.68	−1.733 85	−9.588 79	35.632 259	Me_4Sn	Neat/ C_6D_6	3.54×10^{-3}	20.8
^{119}Sn	8.59	−1.813 94	−10.0317	37.290 632	Me_4Sn	Neat/ C_6D_6	4.53×10^{-3}	26.6
^{123}Te	0.89	−1.276 431	−7.059 098	26.169 742	Me_2Te	Neat/ C_6D_6	1.64×10^{-4}	0.961
^{125}Te	7.07	−1.538 9360	−8.510 8404	31.549 769	Me_2Te	Neat/ C_6D_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_2WO_4	D_2O , 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_2PtCl_6	D_2O , 1.2 M	3.51×10^{-3}	20.7
^{199}Hg	16.87	0.876 219 37	4.845 7916	17.910 822	Me_2Hg^a	Neat	1.00×10^{-3}	5.89
^{203}Tl	29.524	2.809 833 05	15.539 3338	57.123 200	$\text{Tl}(\text{NO}_3)_3$	See lit.	5.79×10^{-2}	3.40×10^2
^{205}Tl	70.476	2.837 470 94	15.692 1808	57.683 838	$\text{Tl}(\text{NO}_3)_3$	See lit.	0.142	8.36×10^2
^{207}Pb	22.1	1.009 06	5.580 46	20.920 599	Me_4Pb	Neat/ C_6D_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^B	D^C
^2H	1	0.0115	1.212 600 77	4.106 627 91	0.2860	15.350 609	(CD_3) $_4\text{Si}$	CDCl_3 $\varphi = 1\%$	0.41	1.11×10^{-6}	6.52×10^{-3}
^6Li	1	7.59	1.162 5637	3.937 1709	-0.0808	14.716 086	LiCl	D_2O , 9.7 m	0.033	6.45×10^{-4}	3.79
^7Li	3/2	92.41	4.204 075 05	10.397 7013	-4.01	38.863 797	LiCl	D_2O , 9.7 m	21	0.271	1.59×10^3
^9Be	3/2	100	-1.520 136	-3.759 666	5.288	14.051 813	BeSO_4	D_2O , 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	$\text{BF}_3 \cdot \text{Et}_2\text{O}$	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	$\text{BF}_3 \cdot \text{Et}_2\text{O}$	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_3NO_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_2O	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_2O , 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_2O , 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	$\text{Al}(\text{NO}_3)_3$	D_2O , 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	$(\text{NH}_4)_2\text{SO}_4$	D_2O , 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_2O , 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_2O , 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_2O , 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_2O , 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_2O , 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_2O , 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	$\text{Sc}(\text{NO}_3)_3$	D_2O , 0.06 M	66	0.302	1.78×10^3
^{47}Ti	5/2	7.44	-0.932 94	-1.5105	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_6D_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_6D_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_2CrO_4	D_2O , 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_2O , 0.82 m	350	0.179	1.05×10^3
^{59}Co	7/2	100	5.247	6.332	42.0	23.727 074	$\text{K}_3[\text{Co}(\text{CN})_6]$	D_2O , 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	$\text{Ni}(\text{CO})_4$	Neat/ C_6D_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	$[\text{Cu}(\text{CH}_3\text{CN})_4][\text{ClO}_4]$	CH_3CN , 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	$[\text{Cu}(\text{CH}_3\text{CN})_4][\text{ClO}_4]$	CH_3CN , 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	$\text{Zn}(\text{NO}_3)_2$	D_2O , 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	$\text{Ga}(\text{NO}_3)_3$	D_2O , 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	$\text{Ga}(\text{NO}_3)_3$	D_2O , 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	$(\text{CH}_3)_4\text{Ge}$	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_3CN , 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^B	D^C
(⁷⁹ Br)	3/2	50.69	2.719 351	6.725 616	31.3	25.053 980	NaBr	D ₂ O, 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 ₂ O, 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 ₂ O, 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 ₂ O, 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 ₂ O, 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	Zr(C ₅ H ₅) ₂ Cl ₂	CH ₂ Cl 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 ₃ CN, sat.	76	0.488	2.87×10^3
⁹⁵ Mo	5/2	15.92	-1.082	-1.751	-2.2	6.516 926	Na ₂ MoO ₄	D ₂ O, 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 ₂ MoO ₄	D ₂ O, 2 M	210	3.33×10^{-4}	1.95
⁹⁹ Tc	9/2	—	6.281	6.046	-12.9	22.508 326	NH ₄ TcO ₄	D ₂ O	12	—	—
⁹⁹ Ru	5/2	12.76	-0.7588	-1.229	7.9	4.605 151	K ₄ [Ru(CN) ₆]	D ₂ O, 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 ₂ O, 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 ₂ O, 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 ₂ O, 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 ₂ O, 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	KSbCl ₆	CH ₃ CN, 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	KSbCl ₆	CH ₃ CN, 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 ₂ O, 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 ₂ O, 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 ₂ O, 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 ₂ O, 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	D ₂ O/H ₂ 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 ₂ O, 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 ₃ CN, 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 ₂ O, 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 ₂ O, 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 ^a	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) ₃	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.

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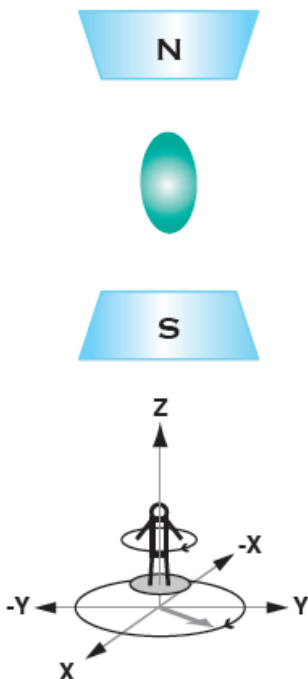
MOST ABUNDANT NMR ACTIVE NUCLEI

Spin = $\frac{1}{2}$
Spin > $\frac{1}{2}$

Quadrupolar

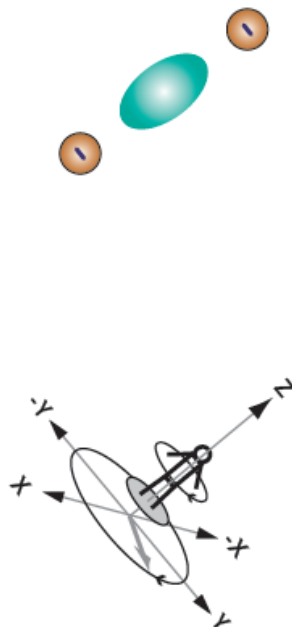
Interação nuclear combinada: magnética e elétrica

NUCLEAR MAGNETIC
DIPOLE MOMENT COUPLES
TO MAGNETIC FIELD

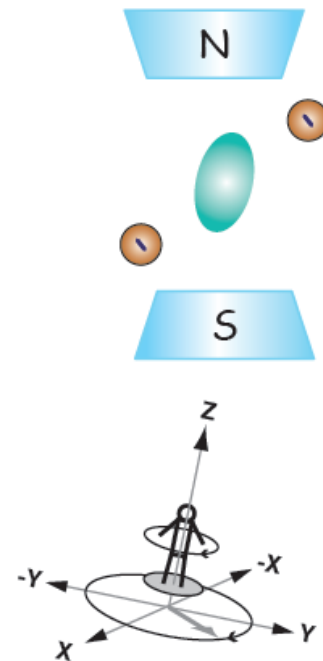


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NUCLEAR ELECTRIC
QUADRUPOLE MOMENT
COUPLES TO ELECTRIC
FIELD GRADIENT



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

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