R — Dipolar Couplings and Nuclear Properties

Contents

1 R Help File

Select one of the buttons below to obtain more information on a specific topic:

Button	Function	Short Description
	OK (p. 11)	Quit R
	R (p. 4)	Calculate a dipolar coupling constant
	Table (p. 5)	Display a table of nuclear properties
	PSE (p. 7)	Display a periodic system of elements
	Help (p. 8)	Display this help file
	Copyright (p. 9)	The obligatory copyright statement
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	Acknowledgements (p. 12)	Contributions to this project
	History (p. 2)	A summary of program changes

1.1 Revision History

1.1.1 Changes in Version 2.3.15 (11.06.2021)

- (Bug) fix: the tables had a wrong magnetogyric ratio for ^{207}Pb; see Table of nuclear properties (p. 5); sorting the table for spin sorts the table for atomic number also.

1.1.2 Changes in Version 2.3.14 (19.05.2021)

- Bug fix: newer versions of Adobe Acrobat (Reader) should be supported for context sensitive help. (I am installing Acrobat only occasionally, hence I am not always able to check.)

1.1.3 Changes in Version 2.3.12 (06.04.2015)

- New feature: created a portable version. Upon start of R, the program checks the entry `portable` in the section `[GENERAL]` of the r.ini file in the program directory. If `portable` equals 0, R expects per user settings and from now on checks the r.ini file in the user's documents directory (subdirectory WSolids). If `portable` equals 1, R keeps using the r.ini file in the program's directory. I.e., changing the portability parameter makes R portable or non-portable.
- New feature: the r.ini file is in the user's document directory, and gets copied there from the application's directory if necessary.
- New feature: Periodic System of Elements (p. 7) displays the frequency of the reference compound (standard) instead of the Larmor frequency.
- New feature: Table of nuclear properties (p. 5) and Periodic System of Elements (p. 7) now display a combo box where the strength of the external magnetic field can be selected or entered. The default value is retrieved from the r.ini file (entry `B0` in the section `[GENERAL]`)
- Bug fix: R did not show up on the task bar and did not close properly.

1.1.4 Changes in Version 2.3.9 (06.03.2014)

- Periodic System of Elements (p. 7): show the sign of the Larmor frequency, as in the Table of nuclear properties (p. 5)
- the main dialog can also be closed using ESC
- added DOIs to references in help file

1.1.5 Changes in Version 2.3.8 (25.05.2010)

- no changes, just to synchronize with associated libraries

1.1.6 Changes in Version 2.3.7 (02.01.2009)

- added Adobe Acrobat PDF file as documentation instead of Windows help file
- Table of nuclear properties (p. 5): included a field option and frequency column in list box

1.1.7 Changes in Version 2.3.3 (29.09.2008)

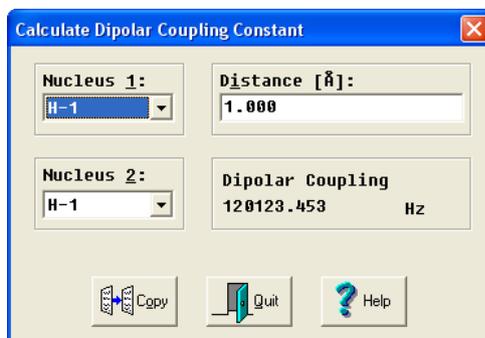- switched from Borland C++ to Microsoft Visual Studio C++ 2008

1.1.8 Changes in Version 2.2.4 (30.04.2004)

- Added a call to ini file to retrieve field strength parameter as default for Periodic System of Elements (p. 7).

- Included and corrected isotopes (p. 5): new Q values from Pyykkö, fixed spin of Nd-145 and U-235 and added U-233; modified to incorporate IUPAC Recommendations 2001.

- Fixed a bug where the hidden main window did not get closed because no closing message was created. (Zombie application)

1.1.9 Version 2.1.1 (23.05.2001)

- First Win32 version.

2 Calculate Dipolar Coupling Constant

Selection of the **R** button invokes this dialog box.

The dipolar coupling constant is defined as:

$$R = \frac{\mu_0}{4\pi} \frac{\hbar}{2\pi} \frac{\gamma_I \gamma_S}{r_{IS}^3}$$

Here, μ_0 is the permeability of vaccuum, $\mathbf{r}_{IS}$ is the internuclear separation, γ_I and γ_S are the magnetogyric ratios of the interacting nuclei, and $\hbar$ is Planck's constant divided by 2π.

To calculate the dipolar coupling constant, follow these steps:

- Select from the two list boxes **Nucleus 1** and **Nucleus 2** the two nuclei constituting the spin pair
- Enter the internuclear separation in Angstrom
- Hit **Enter** to display the calculated dipolar coupling constant
- If required, copy the result to the clipboard by pushing the **Copy** button (or ALT-O). This can be used to **paste** (typically CTRL-V or SHIFT-INSERT) the result into appropriate edit controls
- Exit the dialog by selecting **Quit** (or ESC)

For information on the source of the nuclear data, refer to Table of Nuclear Properties (p. 5).

3 Table of Nuclear Properties


```
Nuclear Properties                                                          ×
  No. Nucleus  Spin  Gamma/1E07    N.A./%      Q/1E-28   Larmor/MHz  Shift-Reference/MHz
   1   H-1     1/2     26.75221    99.9880     0.00000   200.114090      200.114014   ▲
   2   H-2     1        4.10663     0.0115     0.00286    30.718735       30.718719   
   3   H-3     1/2     28.53498     0.0000     0.00000   213.449677      213.449554   
   4   He-3    1/2    -20.38016     0.0001     0.00000  -152.449341     -152.445724   
   5   Li-6    1        3.93717     7.5900    -0.00081    29.451149       29.448952   
   6   Li-7    3/2     10.39770    92.4100    -0.04010    77.777740       77.771904   
   7   Be-9    3/2     -3.75967   100.0000     0.05288   -28.123362      -28.119648   
   8   B-10    3        2.87468    19.9000     0.08459    21.503407       21.499565   
   9   B-11    3/2      8.58470    80.1000     0.04059    64.216011       64.204529   
  10   C-13    1/2      6.72828     1.0700     0.00000    50.329460       50.318707   
  11   N-14    1        1.93378    99.6320     0.02044    14.465214       14.460873   
  12   N-15    1/2     -2.71262     0.3680     0.00000   -20.291149      -20.285091   
  13   O-17    5/2     -3.62808     0.0380    -0.02558   -27.139061      -27.128370   
  14   F-19    1/2     25.18148   100.0000     0.00000   188.364578      188.295303   
  15   Ne-21   3/2     -2.11308     0.2700     0.10155   -15.806435      -15.797593   ▼

  Sort for: │No.              ▼│        Magnetic Field [T]:   │4.700000        ▼│

                      ⬚ Quit              ? Help
```

Selection of the **T** button displays this dialog box which lists nuclear properties for many of the known NMR active nuclei.

The Properties:

- nuclear **spin** quantum number
- magnetogyric ratio, **Gamma**, in units of 10^7 rad s^{-1} T^{-1}
- natural abundance, **N.A.**, in %
- nuclear electric quadrupole moment, **Q**, in units of 10^{-28} m^2
- Larmor frequency, in MHz, at the selected magnetic field strength according to

$$\nu_L = \frac{\gamma}{2\pi} B_0$$

- Shift-reference frequency, in MHz, of the reference compound for that nucleus (standard) at the selected magnetic field strength according to

$$\nu = \Xi \quad \frac{B_0}{2.348661}$$

  using the absolute frequency ratio Ξ as defined by IUPAC [6,7].

Sorting:

By default, the nuclei are listed according to their position in the periodic table of elements (i.e. for increasing mass number). Using the **Sort for:** list box, the display can be sorted alphabetically for the labels of the nuclei, the spin, the magnetogyric ratio (Gamma), the natural abundance, or the nuclear electric quadrupole moment.

Magnetic Field:

The strength of the magnetic field affects the frequency of the reference compound. The following values produce the given values of the ^{1}H NMR frequency of TMS:

B_0 / T	^{1}H frequency of TMS / MHz
2.348661	100.00
4.70037532	200.13
5.874706	250.13
7.049036	300.13
9.397697	400.13
11.746359	500.13
14.095019	600.13
16.44368	700.13
18.792341	800.13
21.141002	900.13
22.315332	950.13
23.489665	1000.13
25.838325	1100.13

Copying Data:

Note that it is possible to high-light parts of the table and to copy the highlighted parts to the clipboard using standard Windows editing techniques (CTRL-INSERT or CTRL-C to copy the selected part).

Modifications:

Most nuclear data have originated from Mason's extremely useful book on *Multinuclear NMR* [1]. The current version of R has been updated according to data from the *IUPAC Recommendations 2001* [6] and *IUPAC Recommendations 2008* [7]. The following data differ from those in reference [1], all magnetogyric ratios are according to [6]:

- the nuclear quadrupole moment values are from the "Year 2001 Q Values" collected by Pekka Pyykkö [3];

- Nd-145 apparently has a spin of 7/2 instead of 5/2 [4,5]. Similarly, U-235 has a spin of 7/2 instead of 5/2 [4,5]. U-233 has been added to the tables [4,5].

- the magnetogyric ratio quoted in *IUPAC Recommendations 2001* [6] for ^{207}Pb was in error, in the 2008 recommendations [7] hidden in a footnote

References:

(1) Joan Mason, *Multinuclear NMR*, Plenum Press, New York, 1987.

(2) A. Laaksonen and R. Wasylishen, *J. Am. Chem. Soc.* **1995**, *117*, 392−400, DOI: 10.1021/ja00106a044.

(3) P. Pyykkö, *Mol. Phys.* **2001**, *99*, 1617−1629, DOI: 10.1080/00268970110069010.

(4) *Quantities, Units and Symbols in Physical Chemistry (IUPAC)*

(5) *CRC Handbook of Chemistry and Physics*

(6) R. K. Harris, E. D. Becker, S. M. Cabral de Menezes, R. Goodfellow, P. Granger:
  - *Pure Appl. Chem.* **2001**, *73*, 1795-1818, DOI: 10.1351/pac200173111795.
  - *Solid State Nucl. Magn. Reson.* **2002**, *22*, 458−483, DOI: 10.1006/snmr.2002.0063.
  - *Angew. Chem.* **2004**, *116*, 2070-2083, DOI: 10.1002/ange.200380015.

(7) R. K. Harris, E. D. Becker, S. M. Cabral de Menezes, P. Granger, R. E. Hoffman, K. W. Zilm, *Pure Appl. Chem.* **2008**, *80*, 59-84, DOI: 10.1351/pac200880010059.

4 Periodic System of Elements

Selection of the **PSE** button displays this dialog box which displays a periodic system of elements.

By setting the magnetic field induction strength, B0, to a specific value in Tesla, this dialog box calculates the corresponding frequency of the reference compound (standard) for the isotopes of the selected element. The default value causes H-1 to have a Larmor frequency of 100.00 MHz.

The default value of the magnetic field is retrieved from the INI file and can be changed there. If there is no INI file or no corresponding entry in the INI file, the default value is 2.34867 T.

For information on the source of the nuclear data, refer to Table of Nuclear Properties (p. 5).

5 Help on Help

The small tool **R** has been designed to provide the user with some information on nuclear properties as they pertain to the field of nuclear magnetic resonance (NMR). **R** relies on the presence of a dynamic link library, **kenuclei.dll,** to perform its duties. The file kenuclei.dll is part of a simulation package, **WSolids**, for the calculation of solid-state NMR spectra.

This program has been developed at the **Department of Chemistry**, **Dalhousie University**, Halifax, N.S., Canada, and **Institut für Anorganische Chemie**, **Universität Tübingen**, Germany.

6 Copyright Statement

7 Disclaimer of Warranty

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8 Quit R

Selection of the **OK** button causes R to quit.

9 Acknowledgements

- P. Pyykkö for sending a preprint of his "Year 2001 Q Values" (P. Pyykkö, *Mol. Phys.* **2001**, *99*, 1617−1629)

- Microsoft for providing Visual C++ 2008 Express Edition for free

- Jordan Russell for making Inno Setup available (http://www.jrsoftware.org/)

- Jochen Kalmbach for demonstrating how to statically link against the Microsoft CRT and thus get rid of VCREDIST_X86.EXE (http://blog.kalmbach-software.de)

- "chicks" for demonstrating in his pdfp PDF tools how to establish Dynamic Data Exchange (DDE) with Adobe Acrobat (Reader) (http://www.esnips.com/web/PDFTools)