The Magpie manual

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Contents

1 Introduction

Magpie (waar staat het voor?) is a program that simualtes an NMR spectrometer environment. It can load sample and pulse sequences, and simulate the outcome of NMR measurements. The goal of the program is to be used in teaching, allowing students a first introduction to practical NMR.

2 Sample definition

Sample files for Magpie need to be in a specific definition. They need to be text files with `.txt` extension.

The file should start with a header:

```
###SAMPLE###
```

Below this, on optional statement regarding the sample amount (concentration) can be made:

```
amount 1
```

In this case, the scaling is set to 1, so it has no effect.

After this, a molecule can be defined. The sample file can hold multiple molecule definitions. Within this block, the spins are set, as well as the overall relaxation times and the J-couplings.

The statements are:

Statement	Input	Description
amount	amount	molecule amount
T1	T1	Overall T1, in seconds (optional)
T2	T2	Overall T2, in seconds (optional)
T2prime	T2prime	Overall T2prime, in seconds (optional)
spin	isotope shift multiplicity	For example: 1H 1.2 3
spin	isotope shift multiplicity T1 T2 T2prime	Spin definition including relation times. These are used in favour of the overall relaxation times, if set. Values can be set empty by an underscore (_)
J	spin1 spin2 strength	Set J-coupling in Hz between two spin indexes. Number order as the spins are defined. For example: J 1 2 9.6
Jmatrix	matrix	Set J-coupling in Hz between all spins in matrix format. Example for two spins: [[0,10],[10,0]], setting 10 Hz coupling. Size needs to be n_spins x n_spins. When used the, regular J statement cannot be used.
pair	isotope shift1 shift2 k amp1 amp2 T1_1 T1_2 T2_1 T2_2	Sets a spin-pair with exchange between them. amp sets the multiplicity. Individual T1 and T2 times can be set, or set to empty by an underscore (_). No J-couplings can be set to these spins.

Either Jmatrix or J statements are allowed. Not both. Spin statements can lack all the relaxation times, or have a _ instead. If a relax time not defined for a spin, it needs to use the global molecule relaxation time. These are also optional, but if they lack, the individual spin lifetimes need to be all there.

An example definition could be the following sample:

```
###SAMPLE###
amount 1
###MOLECULE###
amount 0.1
T1 5
T2 0.5
T2prime 10
```

```
spin 1H 1.2 3
spin 1H 3.6 2
J 1 2 7
```

Here we set a two spin system, with shifts 1.2 and 3.6 ppm, multiplicities 3 and 2. There is a 7 Hz J-coupling between the spins. All nuclei have the same relaxation times, set at 5, 0.5 and 10 s for T1, T2 and T2prime respectively. The overall intensity scaling is set at 1, and the molecule itself has scaling 0.1.

A more complicated sample could be ethanol:

```
###SAMPLE###
amount 1
###MOLECULE###
amount 0.98
T1 5
T2 0.5
T2prime 10
spin 1H 1.226 3
spin 1H 3.692 2
spin 1H 2.605 1 _ 0.01 0.1
J 1 2 7
###MOLECULE###
amount 0.01
T1 5
T2 1
T2prime 10
spin 1H 1.224 3
spin 1H 3.692 2
spin 1H 2.605 1 _ 0.01 0.1
spin 13C 18.1 1 _ _ 7
J 1 2 7
J 1 4 125
###MOLECULE###
amount 0.01
T1 7
T2 1
T2prime 10
spin 1H 1.226 3
spin 1H 3.692 2
spin 1H 2.605 1 _ 0.01 0.1
spin 13C 57.8 1 _ _ 7
```

```
J 1 2 7
J 2 4 125
```

Here we set three molecules: with no 13C nucleus, and both options with a single 13C nucleus (the 13C-13C variant is too low in intensity to care about). The amount of the molecules is set to follow the natural abundance. For the OH peak (at 2.6 ppm), a separate set of relaxation times is set, as to have a shorter T2 and T2prime, to include the fact that this signal is usually exchanging causing line broadening. J-couplings are ste between the 1H nuclei of the CH_3 and CH_2 groups, as well as between the 13C nuclei and their directly bonded 1H nuclei.

3 Pulse sequence definition

4 Data output

5 Simulation background

Magpie uses a classical simulator, so no quantum effects are included. J-couplings are therefore included only as their weak coup;ling limit, and no coherence between the J-states exists.

6 Contact

To contact the `magpie` team write to `ssnake@science.ru.nl`.