

# **Chapter 15**

## **IRMA2**

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## 15.1 Introduction

This manual describes the use and operation of the IRMA2 package. The IRMA procedure was devised for an accurate determination of proton-proton distances from 2D NOE intensities. The most important aspect is the use of full cross-relaxation rate matrices in the procedure which allows a proper treatment of spin diffusion in the interpretation of the NOE intensities. The flow chart of the IRMA procedure is given in Figure 1. The method has been described in detail in references (1,2), but a brief description will be given in this introduction.

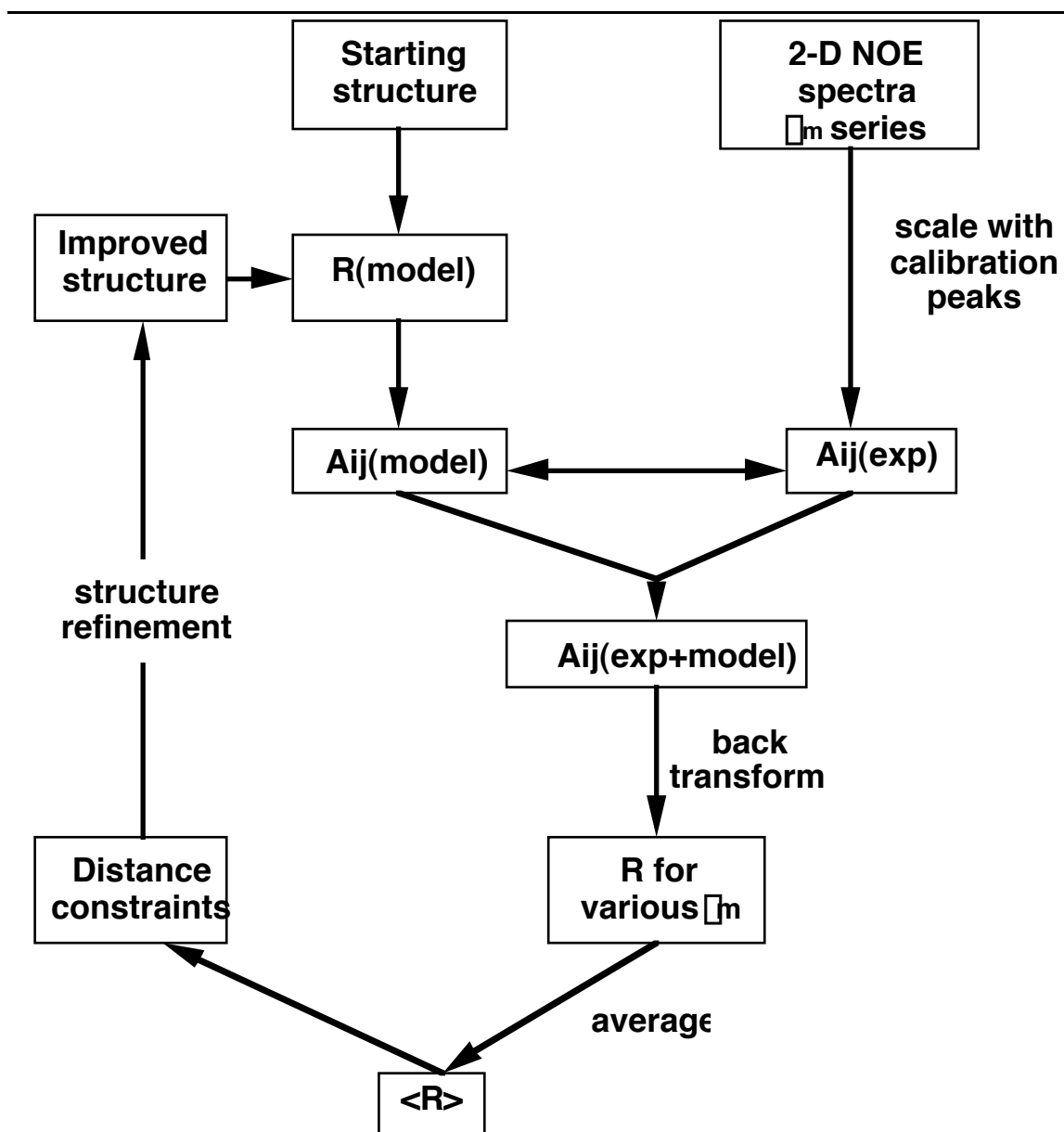


Figure 1. Schematic presentation of the IRMA procedure

The NOE intensities measured for a series of mixing times form the major input of IRMA. In principle this would be sufficient for distance determination. However, experimental data are

incomplete due to overlapping peaks and assignment problems and it becomes impossible to convert the experimental NOE intensities directly into distances. But these data can be supplemented by theoretical NOE intensities calculated from a model structure and the back transformation to distances is then possible. Distances obtained from the model structure are used to calculate spectral density functions and from these the cross-relaxation matrix **R** is constructed. For the equations used see (1-2). This cross-relaxation matrix is used to calculate a theoretical NOE intensity matrix **A(model)** with the same mixing times as the experimental ones (**A(exp)**). **N.B.** It is our experience that, although in principle one mixing time would be sufficient, a set of 4 or more mixing times gives better results and an idea of the accuracy of the whole procedure. After calculation of the theoretical NOE matrices, they are “mixed” with the scaled corresponding experimental ones in the sense that wherever there is an experimentally observed intensity the theoretical intensity will be replaced by this value. The mixed NOE matrices **A(model+exp)** can now be transformed into cross-relaxation matrices **R(t<sub>m</sub>)**. In theory the matrices for all mixing times should be equal. In practice they are almost equal and the standard deviation calculated when averaging these matrices serves as a measure for the accuracy of the procedure. It is used to define upper and lower bounds on the distance constraints. These constraints obtained from the average **R** can be used in a structure refinement procedure. This can be: distance geometry, molecular dynamics, simulated annealing... The user is free to choose his favourite method of structure refinement, since **NO** refinement program is part of the IRMA2 package. When you have obtained an improved structure for your molecule, the whole IRMA cycle can be repeated using this new structure as starting model. IRMA2 also allows the calculation of the theoretical NOE intensities from a set of structure or a MD trajectory. This option can be useful when dealing with an “ensemble” of structure or with local mobility. The iteration should stop when the structure is in agreement with the experimental data. A measure of this agreement can be obtained from an NMR R-factor as proposed in reference (5).

The effects of motions can be included in the interpretation of the NOE intensities and have been implemented in this latest version of IRMA. Aromatic ring flip, methyl rotation and fast local motions can be incorporated in the calculations:

- aromatic ring flip is described by averaging the cross-relaxation rate elements of the protons which exchange position. This approach can also describe a symmetrical exchange problem. This corresponds to  $\langle r^{-6} \rangle$  averaging.
- methyl rotation is usually faster than the overall tumbling of the molecule and the  $\langle r^{-6} \rangle$  averaging is no longer correct. The averaging of the position should occur according to  $\langle r^{-3} \rangle$ . For a detailed description of the theory see (3-4). In case of a slow rotation of the methyl group an  $\langle r^{-6} \rangle$  averaging can be used.
- Fast local motions can be included via an order parameter  $S^2$  according to the model free approach of Lipari and Szabo. This order parameter varies between 1 and 0 and is a measure of the mobility of the interproton vector. Averaging of the distances from a set of structures or from a MD trajectory also takes into account local mobility. The two approaches should be combined for a complete description of local mobility.

The implementation and the use of IRMA will be described in the next sections. A description of the different parameters and procedures will also be given.

## 15.2 Implementation

In this section the implementation of the IRMA2 package is described for VAX/VMS systems and for UNIX operating systems.

### 15.2.1 Installation under VAX/VMS

After you have copied the files from tape (BACKUP or COPY) you can set up your own IRMA2 environment. This is done by editing the command file IRMA.COM and adapting the third line to your own situation. After this you execute this command file and the environment is defined together with some symbols for running the IRMA procedure.

The compilation and linking of the programs is done by using the command file INSTAL.COM. This command file executes the two following procedures COMPILE.COM and LINK.COM. These two procedure are based on our NMR software and you should modify them if you don't have the entire Triton software. You should replace NMRSUBLIB with NMRSUBS which is included in the IRMA2 package. The program MXSPC2 is based on subroutine from the Triton software and can't be linked without this latter.

Running IRMA2 is now simple: you create the files needed as input (see 15.4) and run the command procedures by typing the symbols which have been defined with irma.com.

Concluding:

To install :

```
$ edit [.PRGRMS]COMPILE.COM
$ edit [.PRGRMS]LINK.COM
$ @INSTAL
$ edit [.CMMNDS]IRMA.COM
```

For a test :

```
$ SET DEF [.TEST1]
files (remove protection):
test#.inp -- example input for IRMA created with MATRIX
test#.mdh -- coordinates
test#.noe -- noes (with intensities from 8 mixing times)
test#.ord -- order parameters
$ @[-]IRMA.COM
$ SETUP
molecule name: test
$ @[-]THENOES
moleculename: test
directory: []
coordinates: test.mdh
order par. : test.ord
mixing times: 8
$ @THENOES.JOB
$ @[-]CRENOES
moleculename: test
directory: []
coordinates: test.mdh
noes: test.no
mixing times: 8
$ @[-]MERGNOES
moleculename: test
directory: []
coordinates: test.mdh
```

```

order par. : test.ord
mixing times: 8
$ @MERGNOES.JOB --- needs privilege to open >20 files
                    (modify/fillm=30)

$ @[-]MXRDIS
$ type DISTEST.LIS
$ @[-]MXRFAC
the same output must be present in [.EXAMPLEOUTPUT]

```

For a normal run :

```

$ @[-]IRMA
$ SETUP
$ MATRIX          -- TEST.INP created (there is already a copy!)
$ THENOES         -- calculation of theoretical NOEs
$ submit THENOES.JOB
$ CRENOES         -- experimental NOE matrices are created
$ submit or execute MXCREX.JOB
$ MERGNOES        -- mixing of exp. and theo. NOEs and back
                    transformation
$ submit MERGNOES.JOB
$ MXRDIS          -- or alternatively MAKENOE
$ type DISTEST.LIS -- the IRMA output,
                    which must be converted for DG or restrained MD
$ MXRFAC          -- calculate some R-factors

```

### 15.2.2 Installation under UNIX

Setting up IRMA2 in a UNIX environment is not really different from the situation in section 15.2.1. The files are copied from tape to disk with the **'tar xv'** command. You will notice the existence of a file **'readme'** and it is advisable to read this file before you continue. The compilation and linking of the programs is performed by executing the makefile with **make**, but you will first have to modify this makefile to adapt it to your environment. After this you will have to modify the file **irma** to adapt it to your environment. You can now run IRMA2.

Concluding:

To install:

```
% Make
```

To setup:

```
% alias irma source ~3vision/nmr/smx/prgrms/irma2/bin/irma
```

To start:

```
% irma ---- directories and alias defined
% setup ---- define molecule name
% remind ---- show definitions and procedure
```

Before you start you have to create several files in your current directory.

You need:

- the experimental NOEs in your NMR directory in the format of a result file of BUILDUP (named mol.noe).
- a coordinate file in MD format with only protons (mol.mdh)

If you have the all atom file, you must extract only the protons from this list. This file is needed to create the input file and is used in the procedure THENOES to create the relaxation matrix. If you want to calculate NOEs from several structures or from an MDtrajectory, you can use the procedure THENOESAD. You need therefore a file containing the protons coordinates for all structures. This file can

be created from GROMOS coordinates or trajectory file with the program CONVER.

First give the name of your molecule >

```
% setup == setup.csh
```

Next define the input file for all IRMA programs >

```
% mxmat == matrix.csh
```

Then start the IRMA procedure. The procedure is divided into three stages:

- creation of theoretical NOE matrices on basis of the model >

```
% mxthe == thenoes.csh > thenoes.job created ( batch it)
```

or

```
% mxade == thenoesad.csh > thenoesad.job created ( batch it)
```

- creation of the experimental NOE matrices >

```
% mxcre == crenoes.csh > mxcrex.job created ( run interactive)
```

- merging of theory and experiment and calculation of new distances >

```
% mxmer == mergnoes.csh > mergnoes.job created ( batch it)
```

Two additional procedures allow one to get the distances from the distances matrix (mxrdis) and to calculate R-factors (mxrfac). The constraints are found on the file dismol.lis. This file can be used after transformation as input in a restrained MD or DG calculation; the MD and DG programs should be obtained separately.

Additional programs:

- mx2spn ... calculate a NOE matrix with the 2spin approximation; the result can be compared with the output of mx2dno in the procedure mxthe.

- mxspc2 ... calculate a spectrum on basis of a NOE matrix in the SMX format, the chemical shifts must be on a separated file.

## 15.3 Procedures in IRMA2

There are ten different procedures (VAX/VMS command files or UNIX script files) in IRMA2. These procedures are **setup**, **matrix**, **thenoes**, **thenoesad**, **crenoes**, **mergnoes**, **mxrdis**, **mxrfac**, **mx2spn**, **mxspc2**. The procedures **matrix**, **mxrdis** and **mxspc2** are run interactively, **crenoes** can be run interactively, the other procedures should be run in batch mode. Before using these procedures you should first define your IRMA2 environment with:

```
@[*irma2.cmmnds]irma.com (VAX/VMS)
source */irma2/cmmnds/irma (UNIX)
```

### 15.3.1 Setup

This procedure should be run first. It defines or modify the default molecule name for the run. This name is used in every procedure to identify file names.

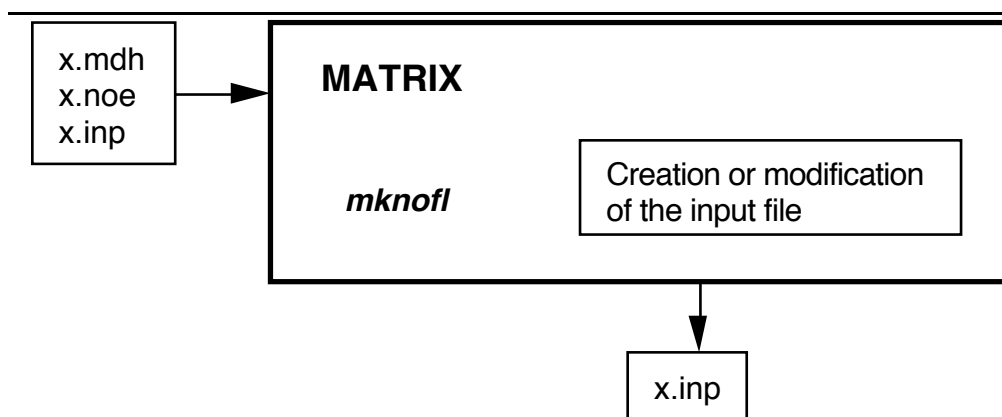
### 15.3.2 Matrix

**Matrix** create or modify the input file (x.inp). File names are directly asked by the program. To create the IRMA2 input file you need an all protons coordinate file (x.mdh) and a NOE result file (x.noe). The numbering of the atoms should be consistent in both files.

call:           matrix or mxmat

input:          proton coordinates file (x.inp)  
                result file with experimental NOEs (x.noe)

output:         IRMA2 input file (x.inp)



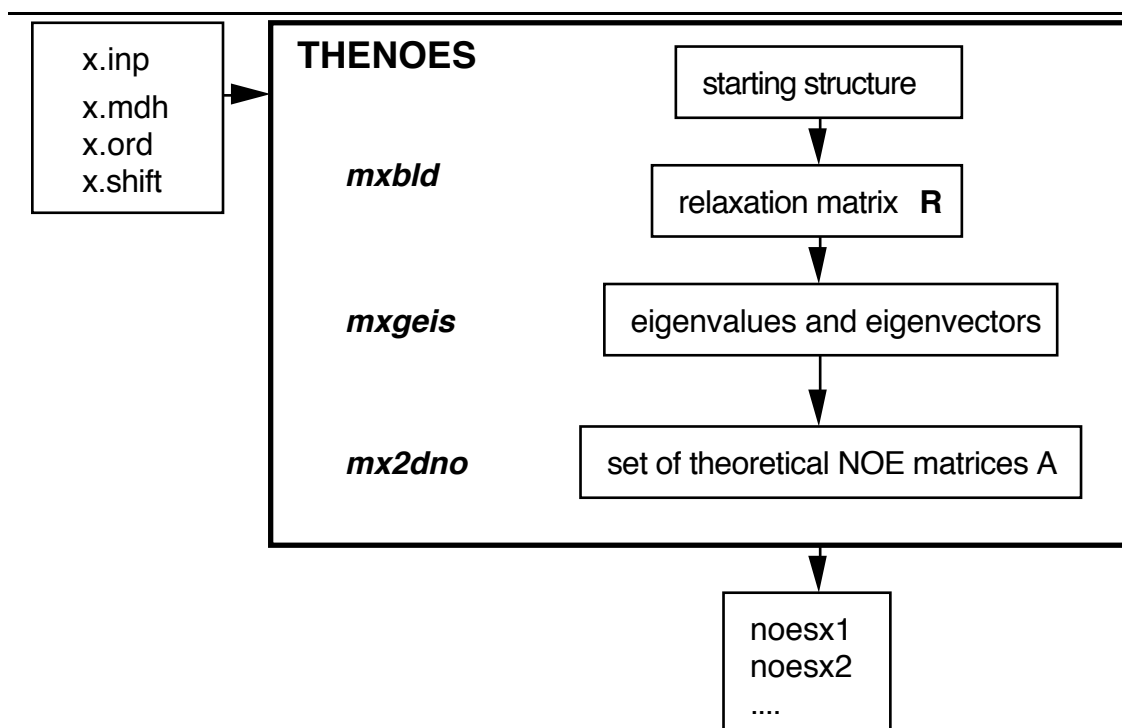
### 15.3.3 Thenoes

This procedure creates a job file called **thenoes.job**. It calculates theoretical NOE intensity matrices from one structure. This procedure is rather time consuming and should be run in background.

call:            thenoes or mxthe

input:           IRMA2 input file (x.inp)  
                  proton coordinates file (x.mdh)  
                  order parameter matrix (x.ord) (option)  
                  chemical shift file (x.shift) (option)

output:           set of theoretical NOE matrices (noesx1, noesx2, ...)



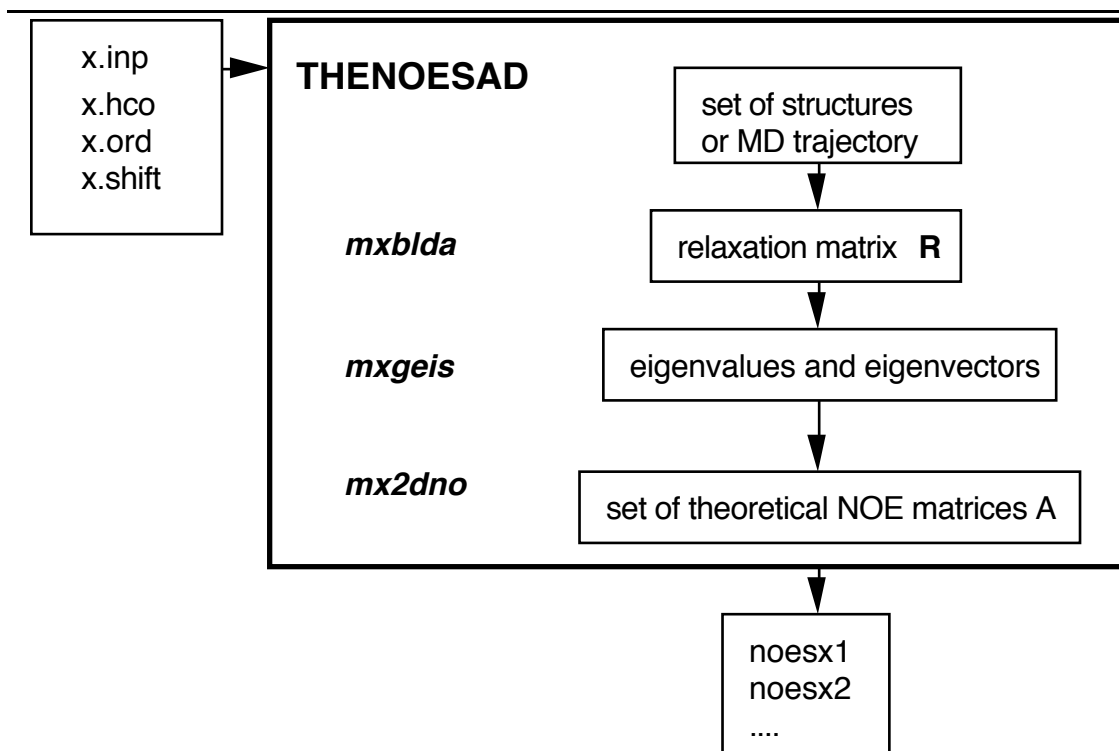
### 15.3.4 Thenoesad

This procedure creates a job file called **thenoesad.job**. It calculates theoretical NOE intensity matrices from a set of structures or from an MD trajectory. This procedure is rather time consuming and should be run in background.

call:            thenoes or mxthe

input:           IRMA2 input file (x.inp)  
                  proton coordinates trajectory file (x.hco) (binary)  
                  order parameter matrix (x.ord) (option)  
                  chemical shift file (x.shift) (option)

output:           set of theoretical NOE matrices (noesx1, noesx2, ...)



### 15.3.5 Mx2spn

This procedure creates a job file called **mx2spn.job**. It calculates theoretical NOE intensity matrices using a two spin approximation.

call:           mx2spn

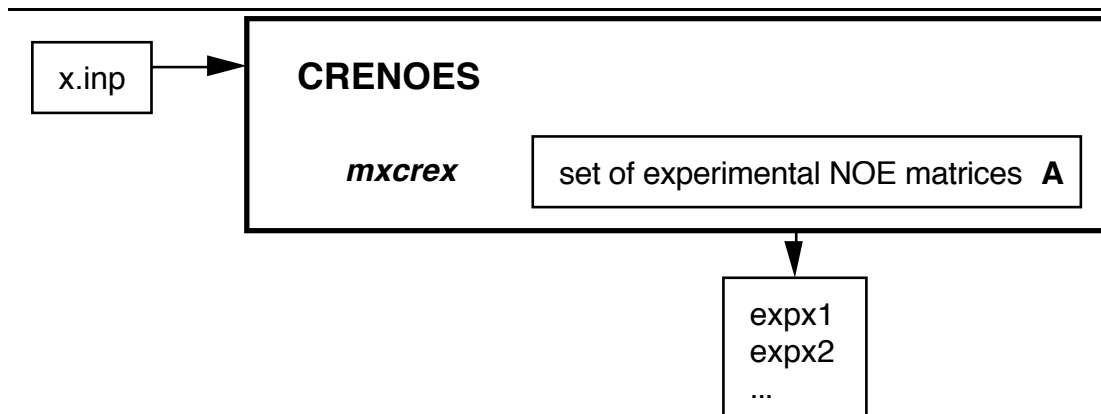
input:           IRMA2 input file (x.inp)  
                   proton coordinates file (x.mdh)  
                   order parameter matrix (x.ord) (option)  
                   chemical shift file (x.shift) (option)

output:          set of theoretical NOE matrices (noesx1, noesx2, ...)

### 15.3.6 Crenoes

This procedure creates a job file called **mxcrex.job**. It creates experimental NOE intensity matrices.

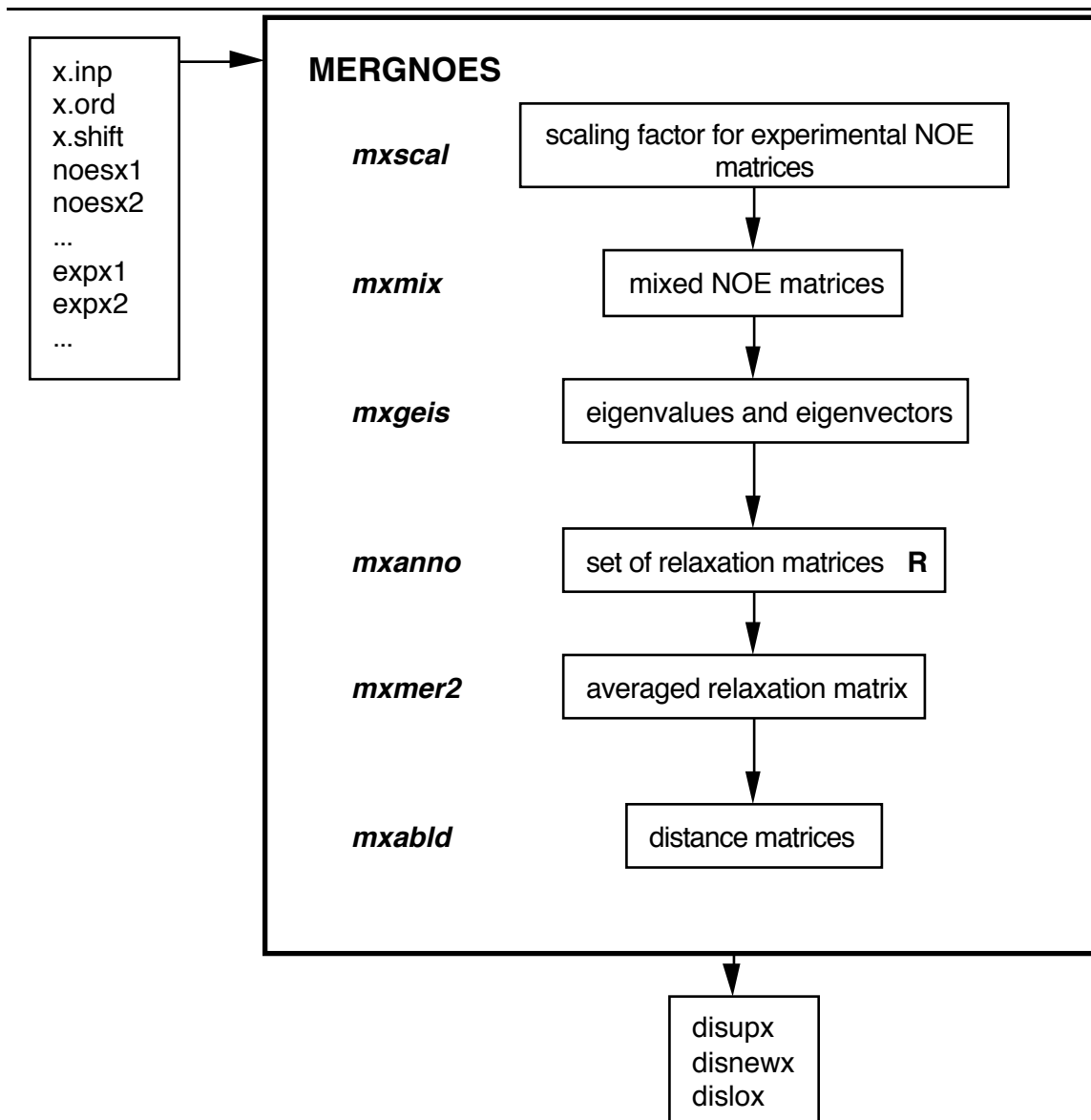
call:            crenoes or mxcre  
input:           IRMA2 input file (x.inp)  
output:          set of experimental NOE matrices (expx1, expx2, ...)



### 15.3.7 Mergnoes

This procedure creates a job file called **mergnoes.job**. This is the major part of IRMA, it mixes the experimental and theoretical NOE matrices and transforms them back into distances. This is the most time consuming part of IRMA and should be run in background.

call:            mergnoes or mxmer  
input:           IRMA2 input file (x.inp)  
                  order parameter matrix (x.ord) (option)  
                  chemical shift file (x.shift) (option)  
                  theoretical and experimental NOE matrices (noesx%, expx%)  
output:          upper bound distance matrix (disupx)  
                  IRMA distance matrix (disnewx)  
                  lower bound distance matrix (dislox)



### 15.3.8 Mxrdis

This procedure creates an IRMA distance file from the distance matrices (output mergnoes). No corrections for pseudo-atoms are included in this procedure. Proton identification strings from the input file are used in this file.

call:           mxrdis

input:          IRMA2 input file (x.inp)  
                distance matrices (disupx, disnewx, dislox)

output:         IRMA distance file (disx.lis)

### 15.3.9 Mxrfac

This procedure run interactively and calculates a set of R-factor using eight different definitions. This gives an idea of the correspondence between experimental and theoretical NOEs. Experimental intensities can be read from the experimental matrices or from the input file. This procedure can also calculate R-factors from a subset of NOEs. If the latter option is used, peak numbers for the subset are read from an additional file of which the name is required by the program. This file contains a title (a80), the number of peaks which will be read in this file (free) and for each peak two proton numbers as identification (free).

call: mxrfac

input: IRMA2 input file (x.inp)  
theoretical NOE matrices (noesx%)  
experimental NOE matrices (expx%) (option)

output: R-factor file (x.rfac)

### 15.3.10 Mxspc2

This procedure simulates theoretical NOE spectra. It also allows a visual inspection of any matrix. This procedure creates an SMX file which can only be inspected with the Triton software. File names and parameters are asked interactively by the program.

call: mxspc2

## 15.4 Important files in IRMA2

In this section the important files in IRMA2 are described. These are:

- the general IRMA input file
- the proton coordinates file
- the proton coordinates trajectory file
- the result file
- the chemical shift file
- the order parameter matrix
- the set of experimental NOE matrices
- the set of theoretical NOE matrices
- the file with the R-factor values
- the file with the IRMA distances.

### 15.4.1 IRMA2 input file

This file contains the experimental NOE intensities and all the necessary information for the calculations and for the handling of the protons. It can be created or modified by the procedure **matrix**. You need therefore a proton coordinates file and an experimental NOE file. This input file is used by every program in IRMA2. The format is the following:

- |      |        |  |
|------|--------|--|
| (1)  | (a80)  | title  |
| (2)  | (free) | spectrometer frequency (Hz)  |
| (3)  | (free) | correlation time for overall tumbling in seconds   |
| (4)  | (free) | additional leakage rate for the diagonal (1/s)   |
| (5)  | (free) | additional diagonal relaxation contribution and correlation time for methyl groups. The additional relaxation contribution is calculated in the procedure matrix from the overall and methyl rotation correlation times.   |
| (6)  | (free) | scaling factor for the proton coordinates (IRMA works in Å)  |
| (7)  | (free) | standard deviation factors (sdfac 1 and 2). These factors are used 1) when averaging the relaxation matrices in the procedure mergnoes: all the relaxation matrix elements which are outside the averaged value $\pm$ (sdfac1*standard deviation) will be skipped, 2) when calculating upper and lower limits after "filtering of the noisy data": the remaining relaxation matrix elements are averaged and this averaged value $\pm$ (sdfac2*standard deviation) determine the upper and lower limits. |
| (8)  | (free) | logical for the inclusion of the chemical shifts in the calculation of the relaxation matrix elements.   |
| (9)  | (free) | logical for the inclusion of the generalised order parameters in the calculation of the relaxation matrix elements.  |
| (10) | (free) | three logicals indicating the way the theoretical, experimental and order parameter matrices are written (T: form., F:uniform.)  |
| (11) | (free) | flag for the handling of the experimental NOE matrices:<br>1: matrices will be symmetrised<br>0: no change   |
| (12) | (free) | flag for selection of experimental NOE intensities:<br>-1: negative values will be skipped<br>0: no skip<br>+1: positive values will be skipped  |
| (13) | (free) | flag defining the weighting factors for the averaging of the relaxation matrices(procedure mergnoes):  |

		0: experimental NOE intensities
		1: mixing time
		2: all weighting factor equal to 1
(14)	(free)	logical for the treatment of the overlapping peaks: T: keep them and divide the intensities by two F: skip them
(15)	(free)	type of distance averaging if procedure thenoesad is used: 3: $\langle 1/r^{**3} \rangle$ 6: $\langle 1/r^{**6} \rangle$
(16)	(free)	type of scaling of theoretical vs experimental NOEs 0: using reference peaks 1: using all peaks, separately for each mixing time 2: using all peaks over all mixing times 3: using intra residue peaks, separately for each mixing time 4: using intra residue peaks over all mixing times 5: using inter residue peaks, separately for each mixing time 6: using inter residue peaks over all mixing times 7: separate scaling for intra and inter residue peaks, separately for each mixing time 8: separate scaling for intra and inter residue peaks over all mixing times
(17)	(free)	number of reference peaks
(18)	(free)	proton numbers (IRMA internal numbering) for first reference peak
....		
(n)	(free)	two flags for the type of averaging of the methyl and aromatic groups (information only used in procedure matrix).
(n+1)	(free)	number of protons
(n+2)	(9i5,4x,23a)	information for the first proton about the type of averaging and proton identification string. Nine parameters are given for each proton. The first three indicates the type of averaging (motion) and the last six give the proton number (IRMA internal numbering) and the numbers of the eventual averaging partners. first parameter: type of averaging 0: no averaging 1: $\langle 1/r^{**6} \rangle$ averaging (aromatic flip or slow motions) 2: same as 1, but for this proton an additional number is given in the last six parameter which indicates the number of the other type of proton also present on the same aromatic ring. Relaxation rates between these protons should not be averaged 3: $\langle 1/r^{**3} \rangle$ averaging with matrix contraction (methyl rotation or fast motions) 4: $\langle 1/r^{**3} \rangle$ averaging without matrix contraction second parameter: status of the proton 0: not yet encountered 1: already encountered, is part of an averaging process 2: same as 1, in addition will be skipped for matrix contraction third parameter: number of averaging partners of which the number will be read in the following columns
....		
(n')	(free)	number of mixing times
(n'+1)	(free)	mixing times in seconds
(n'+2)	(free)	number of experimental data (per mixing time)
(n'+3)	(2i5,2x,12(1pe10.3))	peak identification (proton numbers (IRMA internal numbering) and experimental NOE intensities for the buildup

series.

### 15.4.2 The proton coordinates file

This file contains the proton names, numbers and coordinates. The format of this file is strict. Names are only used in the procedure **matrix**. Methyl and aromatic groups will only be recognised in **matrix** if GROMOS names are used. Protons coordinates are read in the procedure **theno**es (program **mxbl**d). The numbering of the protons in this file should correspond with the numbering in the NOE result file. The three protons of the methyl groups and the two equivalent protons of the aromatic groups are assumed to be in following order in this file. If methyl rotation and aromatic ring flip are not included in the calculations the order of these protons is no more important. The format of this file is the following:

(1)	(a80)	title
(2)	(i5)	number of protons in the file
...		
(n)	(i5,2a5,i5,3f8.3)	residue number, residue name, proton name, proton number, x, y, z

### 12.4.3 The proton coordinates trajectory file

This file contains only proton coordinates from a set of structures or from a MD trajectory and is unformatted. It is used in procedure **theno**esad (program **mxbl**da) for calculation of theoretical NOE intensities from a set of structures or from a molecular dynamics trajectory. It contains the following information:

- title
- number of records(structures) in the file (nrec)
- number of protons per record (nhtot)
- for each record: x(1), y(1), z(1), ... , x(nhtot), y(nhtot), z(nhtot)

### 12.4.4 The result file

The result file contains the information on the experimental NOE intensities. It contains a header section, followed by peak information. For each peak two lines (i.e. two Fortran read/write statements) are used. Note that the actual length of the first of these two lines depends on the number of mixing times.

format of the result file:

(1)	(a80)	title
(2)	(i5)	file identification number(not used in IRMA)
(3)	(i5)	NTAPE = number of mixing times = number of NMR files
(4)	(16(1x,1pe10.3))	mixing times
(5)	(2(1x,1pe10.3))	reference rate, reference distance (not used in IRMA)
(6)	(a80)	name of first NMR file (not used in IRMA)
(7)	(a80)	name of second NMR file
....		
(n)	(5(1x,i4 17(1x,1pe10.3))	I, IARRAY(I), JARRAY(I), IARRY2(I), JARRY2(I) RATE(I), YV(1...NTAPE,I),

(n+1)	(1x,11,a1, 2(1x,i4), 1x,a)	SUMMY(I), DELLY(I), SUMMX(I), YFIRR(I) HANDLD(I), PKFLAG(I), IPEAK1(I), IPEAK2(I), PKID(I)
-------	----------------------------------	---

meaning of the variables:

I	peak number(not checked on reading)
IARRAY...JARRY2	channel numbers defining rectangle around peak (not used in IRMA)
RATE	rate defined by fitted buildup curve (not used in IRMA)
YV	array of peak volumes (function of mixing time)
SUMMY YFIRR	data defining fitted buildup curve (not used in IRMA)
HANDLD	logical indicating whether the buildup curve has been fitted or not (not used in IRMA)
PKFLAG	character indicating quality of buildup fit; set by user. (Checked by IRMA, if bad ('b' or 'B') theses buildup data will be skipped)
IPEAK1,IPEAK2	two identification numbers (not used in IRMA)
PKID	peak identification string. Proton numbers and names are used in IRMA. In the name, only the last number is important. If a name ends with a 0 the corresponding peak is assumed to consist of two overlapping peaks and the intensity of these peaks will be divided by two when entering IRMA. If the proton number is 0, the peak is consid- ered as unassigned and will also be skipped when entering IRMA. This string is read in the following format : 2(i5,2a5,i5) (residue number1, residue name1, proton name1, proton number1, residue number2, residue name2, proton name2, proton number2).

### 15.4.5 Chemical shift file

This file contains information about the chemical shifts, the additional diagonal relaxation rates and the line widths. Chemical shifts can be used in the procedure **themoes**, **themoesad** and **mergnoes** to calculate relaxation matrix elements and distances from these elements (in **mergnoes**). The additional diagonal relaxation rates are used in the same way. If the latter are equal to 0, the default value given in the input file will be used. Chemical shifts and line widths are also used for the simulation of NOE spectra. Only protons for which information is available are found in this file. The format of this file is the following:

(1)	(a80)	title
(2)	(free)	number of protons for which information will be read from this file
(3)	(free)	proton number (IRMA internal numbering), chemical shift, additional diagonal relaxation rate, line width
....		

### 15.4.6 Generalised order parameter matrix

This matrix has the size of the matrix after contraction, i.e. each methyl group is treated as one entry, and contains values for the generalised order parameters for each proton-proton contacts. These values vary between 1 and 0 and are obtained from a free molecular dynamics simulation in water. The matrix can be either formatted (8(1pe10.3)) or unformatted.

### **15.4.7 Theoretical and experimental NOE matrices**

These matrices contains the theoretical and experimental NOE intensities. Their size depends on whether or not methyl groups are treated as one entry due to fast rotation. The matrices can be either formatted (8(1pe10.3)) or unformatted.

### **15.4.8 R-factor file**

This file contains R-factor values calculated from experimental and theoretical NOE intensities. Result for eight different R-factor definitions are given in this file. The different definitions can be found in this output file.

### **15.4.9 IRMA distance file**

This file created by the procedure **mxrdis** lists the IRMA distances. No pseudo atom correction are added and the proton identification strings are taken from the IRMA2 input file. If IRMA fails to calculate a distance for one constraint, 999 and 0 Å will be given as upper and lower distance. Due to the way of averaging of the relaxation matrix elements in the procedure **mergnoes**, it is possible that IRMA fails to calculate upper bound distances. In such a case the upper distances will be set to 999 Å.

## 15.5 Programs

All the programs which are part of the IRMA2 procedure are described in this section. The dimensions are defined as parameters in an include file called **noere.inc**. A major part of the parameters and arrays are declared as common blocks and can be found in an include file called **noecom.inc**. Every program must be linked with the IRMA2 library **noerelib** and with a Triton library. (command "clnmr" in link.com). If you don't have the entire Triton software, all the programs except **mxspc2** can be linked with the **nmrsubs** library which is part of the IRMA2 package.

### 12.5.1 MKNOFL

```
=====
c
c PROGRAM : MKNOFL
c -----
c VALID   : IRMA2
c VERSION : 900730
c PURPOSE : create the input file for the IRMA
c CALL    : MKNOFL
c
c REFER.  : -
c
c AUTHOR  : Alexandre Bonvin
c          Laboratory of Organic Chemistry
c          Padualaan 8 , 3584 CH Utrecht, The Netherlands
c
c
c DESCRIPTION
c -----
C   This program generate a NOE data file containing the
C   information for the IRMA.
C   The program reads a result file containing the
C   experimental data; this a result file from BUILDMAN. It also
C   needs an all proton file (actually in GROMOS format).
C
C FILES   :
C
C Output file :
C   - title
C   - spectrometer frequency (FREQ)
C   - overall correlation time (TAUC) and correlation for methyl rotation
C   - additional leakage rate for the diagonal (ROSTARO)
C   - additional diagonal relaxation contribution for methyls (RMETH)
C   - scaling factor for the coordinates (DISFAC)
C   - standard deviation factor for upper and lower distances (SDFAC)
C   - logical for the inclusion of a shift list (SSHIFT)
C   - logical for the inclusion of the order parameters (SPARA)
C   - logicals indicating the way the matrices are written (LEXP,LNOE,LS2)
C   - symmetrize experimental NOE matrices 0=no 1=yes (ISYEXP)
C   - skip exp NOEs : -1 neg., 0 noskipp, 1 pos. (ISKEXP)
C   - type of averaging of the relaxation matrices : (IAVRMX)
C     0=exp NOE intensities
C     1=mixing times
C     2=none (all weights = 1 )
```

```

C - skip unassigned stereospecific (SKIPP) T/F
C - type of averaging of the distances when several structures
C   are used (NAVECO) 6 : <1/dis**6> 3 : <1/dis**3>
C - number of reference peaks (NREF)
C - atoms numbers for the reference peaks (1...NREF)
C   (NREF1, NREF2)
C - type of averaging for methyl and aromatic groups (not used, info)
C - total number of protons (NHTOT)
C - data concerning the proton types for the calculations
C   (ITYPAV(1...NHTOT,MAXAVE). For each proton these data consist of:
C   * information about the type of averaging
C   * flag: 0 the atom hasn't yet been encountered
C           1 the atom has already been encountered
C           2 the atom has already been encountered and will be skipped
C   * number of atoms involved in the averaging (NAVE)
C   * (1...NAVE) atom numbers for the averaging
C   * proton identification
C - number of mixing times (NTM)
C - mixing times (TM(1...NTM))
C - number of experimental constraints NEXP
C - (1...NEXP):
C   * NOE1,NOE2: atom numbers, (AEXP,(1...NTM)): experimental
C   NOE intensity for the different mixing times
c
c PARAMETERS :
c
c ALGORITHM :
c
c USE      : subroutines
c
C - RDRES  : reads the result file
C - RDALLH : reads the GROMOS all protons file and generate a
C           pointer list to the beginning of each residue
C - CHKTYP : search for methyl and aromatic group and set the type
C           of averaging for the calculation of the NOEs
c
c EXAMPLE  :
c
c=====

```

## 15.5.2 MXBLD

```

c=====
c
c PROGRAM : MXBLD
c -----
c
c VALID  : IRMA2
c
c VERSION : 900730
c
c PURPOSE : build a relaxation matrix
c
c CALL   : MXBLD
c
c REFER. : Olejniczak, E.T., Gampe, R.T.,Jr. and Fesik, S.W. (1986),

```

c J. Magn. Reson. 67, 28-41  
c Olejniczak, E.T.(1989), J. Magn. Reson. 81, 392-394  
c Masefski, W.,Jr. and Bolton, P.H. (1985),  
c J. Magn. Reson. 65, 526-530  
c Keepers, J.W. and James, T.L. (1984), J. Magn. Reson. 57, 404  
c Macura, S., Huang, Y., Suter, D. and Ernst, R.R. (1981),  
c J. Magn. Reson. 43, 259-281  
c Jeener, J., Meier, B.H., Bachmann, P. and Ernst, R.R. (1979)  
c J. Chem. Phys. 71,4546  
c Solomon, I. (1953), Phys. Rev. 99, 559-565

c  
c  
c AUTHOR : Alexandre Bonvin  
c Laboratory of Organic Chemistry  
c Padualaan 8 , 3584 CH Utrecht, The Netherlands  
c

#### c DESCRIPTION

c -----  
c MXBLD creates a 2D relaxation matrix  
c with relaxation- and cross-relaxation rates  
c for weakly coupled spin-systems  
c from a proton information list. It is possible to mimic  
c kinetic behaviour of methyl groups and/or aromatic flips  
c This is done by averaging in the rows and the columns  
c involved in such a process (for more details see subroutine  
c SRMATAV).

c FILES : unit 1 : proton coordinates file in GROMOS format  
c unit 2 : order parameter file if the effects of fast local  
c motions are included. This file contains a matrix in  
c which the methyl groups are taken as one entry.  
c format : 8(1pe10.3)  
c unit 3 : output file for the relaxation matrix  
c format : 8(1pe10.3)  
c unit 4 : file containing the chemical shifts, additional  
c diagonal leakage rates and the peak width.  
c (for more details see subroutine RDSHFT)  
c unit 5 : standard input file containing all the parameters  
c for the calculation and the information for the  
c averaging (for more details see subroutine READNO)  
c unit 6 : standard output  
c

c PARAMETERS : all parameters in sec, Hz, ppm and Angstrom  
c

c ALGORITHM :

c USE : subroutines READNO (reads input file)  
c RDALLH (reads gromos coordinates)  
c SMKPOI (makes a pointer list)  
c RDS2MX (reads order parameter matrix)  
c RDSHFT (reads chemical shift file)  
c SRMATAV(create the relaxation matrix)  
c SWRMX (write a real\*8 matrix)  
c

c EXAMPLE :

c

=====

### 15.5.3 MXBLDA

=====

```
c
c PROGRAM : MXBLDA
c -----
c
c VALID  : IRMA2
c
c VERSION : 900802
c
c PURPOSE : build a relaxation matrix by averaging over a trajectory
c           or different structures
c
c CALL   : MXBLDA
c
c REFER. : Olejniczak, E.T., Gampe, R.T.,Jr. and Fesik, S.W. (1986),
c           J. Magn. Reson. 67, 28-41
c           Olejniczak, E.T.(1989), J. Magn. Reson. 81, 392-394
c           Masefski, W.,Jr. and Bolton, P.H. (1985),
c           J. Magn. Reson. 65, 526-530
c           Keepers, J.W. and James, T.L. (1984), J. Magn. Reson. 57, 404
c           Macura, S., Huang, Y., Suter, D. and Ernst, R.R. (1981),
c           J. Magn. Reson. 43, 259-281
c           Jeener, J., Meier, B.H., Bachmann, P. and Ernst, R.R. (1979)
c           J. Chem. Phys. 71,4546
c           Solomon, I. (1953), Phys. Rev. 99, 559-565
c
c
c AUTHOR : Alexandre Bonvin
c           Laboratory of Organic Chemistry
c           Padualaan 8 , 3584 CH Utrecht, The Netherlands
c
c
c DESCRIPTION
c -----
c   MXBLDA creates a 2D relaxation matrix
c           with relaxation- and cross-relaxation rates
c           for weakly coupled spin-systems
c           from a proton information list. It is possible to mimic
c           kinetic behaviour of methyl groups and/or aromatic flips
c           This is done by averaging in the rows and the columns
c           involved in such a process (for more details see subroutine
c           SRMATAV).
c
c FILES   : unit 1 : proton coordinates file in binary format containing:
c
c           line 1 ..... title
c           line 2 ..... number of structures in the file
c           line 3   ..number of atoms to be read per structure
c           line 4 ..... x(1),y(1),z(1)....x(nhtot),y(nhtot),z(nhtot)
c                       for structure 1
c           line n+3 ... x(1),y(1),z(1)....x(nhtot),y(nhtot),z(nhtot)
```

```

c           for structure n
c
c           unit 2 : order parameter file if the effects of fast local
c                   motions are included. This file contains a matrix in
c                   which the methyl groups are taken as one entry.
c                   format : 8(1pe10.3)
c           unit 3 : output file for the relaxation matrix
c                   format : 8(1pe10.3)
c           unit 4 : file containing the chemical shifts, additional
c                   diagonal leakage rates and the peak width.
c                   (for more details see subroutine RDSHFT)
c           unit 5 : standard input file containing all the parameters
c                   for the calculation and the information for the
c                   averaging (for more details see subroutine READNO)
c           unit 6 : standard output
c
c
c PARAMETERS : all parameters in sec, Hz, ppm and Angstrom
c
c ALGORITHM :
c
c USE       : subroutines READNO (reads input file)
c             SRDH  (reads proton coordinates and average)
c             SMKPOI (makes a pointer list)
c             RDS2MX (reads order parameter matrix)
c             RDSHFT (reads chemical shift file)
c             SRMATAV(create the relaxation matrix)
c             SWRMX  (write a real*8 matrix)
c
c EXAMPLE   :
c
c=====

```

## 15.5.4 MXGEIS

```

c=====
c
c PROGRAM : MXGEIS
c -----
c VALID   : IRMA2
c VERSION : 900730
c
c PURPOSE : IRMA diagonalisation of the relaxation matrix
c
c CALL    : MXGEIS
c
c REFER.  : -
c
c AUTHOR  : Alexandre Bonvin
c           Laboratory of Organic Chemistry
c           Padualaan 8 , 3584 CH Utrecht, The Netherlands
c
c
c DESCRIPTION
c -----

```

```

c   Program to find the eigenvalues and eigenvectors of
c       a symmetric matrix
c
c   ! the upper triangular part of the symmetric matrix
c   ! is stored in a linear array with a length equal
c   ! ntdmn=maindm*(maindm+1)/2.
c
c FILES   :
c   input
c   unit 5 : default input used in all programs (mknofl)
c   unit 3 : symmetric matrix
c
c   output:
c   unit 2 : eigenvalues and eigenvectors
c   unit 6 : default output
c
c PARAMETERS :
c
c ALGORITHM :
c
c USE       : GIVEIS from the eispack library and
c             the subroutines called from there
c             READNO (read standard input file)
c             SMKPOI (find matrix dimension and make pointer list)
c             SRDMX  (read a real*8 matrix)
c
c EXAMPLE   :
c
c=====

```

## 15.5.5 MX2DNO

```

c=====
c
c PROGRAM : MX2DNO
c -----
c VALID   : IRMA2
c
c VERSION : 900730
c
c PURPOSE : IRMA calculation of the NOE intensities
c
c CALL    : MX2DNO
c
c REFER.  : Olejniczak, E.T., Gampe, R.T.,Jr. and Fesik, S.W. (1986),
c           J. Magn. Reson. 67, 28-41
c           Masefski, W.,Jr. and Bolton, P.H. (1985),
c           J. Magn. Reson. 65, 526-530
c           Keepers, J.W. and James, T.L. (1984), J. Magn. Reson. 57, 404
c           Macura, S., Huang, Y., Suter, D. and Ernst, R.R. (1981),
c           J. Magn. Reson. 43, 259-281
c           Jeener, J., Meier, B.H., Bachmann, P. and Ernst, R.R. (1979)
c           J. Chem. Phys. 71, 4546
c           Solomon, I. (1953), Phys. Rev. 99, 559-565
c

```

```

c AUTHOR : Alexandre Bonvin
c   Laboratory of Organic Chemistry
c   Padualaan 8 , 3584 CH Utrecht, The Netherlands
c
c
c DESCRIPTION
c -----
c   MX2DNO calculates NOE intensities for all interactions (i,j)
c   from a diagonalised relaxation matrix plus eigenvectors
c
c FILES   :
c
c   unit 3 : LINE(1) .....comment
c           LINE(2) etc. ....eigenvalues of the matrix R in the format :
c             FORMAT(8(1pe10.3))
c           LINE(n) .....comment
c           LINE(n+1) etc. ....eigenvectors (horizontal) in the format :
c             FORMAT(8(1pe10.3))
c   unit 5 : standard input file for the IRMA
c
c   unit 6 : standard output file
c
c   unit 11.. : LINE(1) etc. ....content of the NOE matrix in the format :
c             FORMAT(8(1pe10.3))
c
c PARAMETERS : the present maximal dimension is given by MAINDM
c               in noere.inc
c
c ALGORITHM :
c
c USE       : subroutines READNO (read input file)
c             SMKPOI (make a pointer list and find the
c                 matrix dimensions)
c             SRCORR (calculate a correction factor for
c                 the NOE intensities)
c             SWRMX (write a real*8 matrix)
c EXAMPLE   :
c
c=====

```

### 15.5.6 MX2SPN

```

c=====
c
c PROGRAM : MX2SPN
c -----
c VALID   : IRMA2
c
c VERSION : 900730
c
c PURPOSE : IRMA, NOEs intensities with two spins approximation
c
c CALL    : MX2SPN
c
c REFER.  : OLEJNICZAK, E.T., GAMPE, R.T.,JR. AND FESIK, S.W. (1986),

```

c J. MAGN. RESON. 67, 28-41  
c MASSEFSKI, W.,JR. AND BOLTON, P.H. (1985),  
c J. MAGN. RESON. 65, 526-530  
c KEEPERS, J.W. AND JAMES, T.L. (1984), J. MAGN. RESON. 57, 404  
c MACURA, S., HUANG, Y., SUTER, D. AND ERNST, R.R. (1981),  
c J. MAGN. RESON. 43, 259-281  
c JEENER, J., MEIER, B.H., BACHMANN, P. AND ERNST, R.R. (1979)  
c J. CHEM. PHYS. 71, 4546  
c SOLOMON, I. (1953), PHYS. REV. 99, 559-565

c  
c AUTHOR : Alexandre Bonvin and Rolf Boelens  
c Laboratory of Organic Chemistry  
c Padualaan 8 , 3584 CH Utrecht, The Netherlands

c  
c DESCRIPTION

c -----  
c MX2SPN calculates noe intensities for all interactions (i,j)  
c from a relaxation matrix r with the 2spin approximation  
c this approximation is correct for the approach of the  
c mixing time to zero.

c FILES :  
c unit 3 : relaxation matrix  
c unit 5 : standard input file  
c unit 6 : standard output file  
c unit 11.... : output files with the NOE matrices

c PARAMETERS : The present maximal dimension is given by MAINDM in  
c NOERE.INC

c ALGORITHM :

c USE : subroutine READNO (read input file)  
c SMKPOI (generate a pointer list and find  
c matrix dimension)  
c SRCORR (calculate a correction factor for  
c the NOE intensities)  
c SRDMX (read a real\*8 matrix)  
c SWRMX (write a real\*8 matrix)

c EXAMPLE :

c=====

## 15.5.7 MXCREX

c=====

c PROGRAM : MXCREX

c -----  
c VALID : IRMA2

c  
c VERSION : 900903

c  
c PURPOSE : IRMA, creation of a set of experimental NOE matrices

```

c
c CALL   : MXCREX
c
c REFER. : -
c
c AUTHOR : Alexandre Bonvin
c         Laboratory of Organic Chemistry
c         Padualaan 8 , 3584 CH Utrecht, The Netherlands
c
c
c
c DESCRIPTION
c -----
c FILES   :
c
c   unit 5 : standard input file for the IRMA with parameters for
c           the calculation and experimental NOE intensities
c
c   unit 6 : standard output
c
c   unit 41... : output files for the experimental NOE matrices
c
c PARAMETERS :
c
c ALGORITHM :
c
c USE       : subroutines
c
c           READNO (read input file)
c           SMKPOI (generate a pointer list and find the matrices
c                 dimension)
c           SCOREXP(correct experimental NOE intensities)
c           SWRMX  (write e real*8 matrix)
c
c EXAMPLE   :
c
c=====

```

## 15.5.8 MXSCAL

```

c=====
c
c PROGRAM : MXSCAL
c -----
c VALID   : IRMA2
c
c VERSION : 900731
c
c PURPOSE : IRMA, calculate scaling factor between experimental and
c           theoretical NOE matrices
c
c CALL    : MXSCAL
c
c REFER.  : -
c
c AUTHOR  : Alexandre Bonvin

```

```
c Laboratory of Organic Chemistry
c Padualaan 8 , 3584 CH Utrecht, The Netherlands
```

```
c
c
c DESCRIPTION
```

```
c -----
c FILES :
```

```
c unit 5 : standard input file
c
c unit 11... : theoretical NOE matrices
c
c unit 41... : experimental NOE matrices
c
c unit 1 : output file for the scaling factor
c
c unit 6 : standard output file
```

```
c PARAMETERS :
```

```
c ALGORITHM :
```

```
c USE : subroutines
```

```
c
c READNO (read input file)
c SMKPOI (make pointer list and find matrix dimension)
c SRDMX (read a real*8 matrix)
```

```
c EXAMPLE :
```

```
c=====
```

## 15.5.9 MXMIX

```
c=====
```

```
c
c PROGRAM : MXMIX
```

```
c -----
c VALID : IRMA2
```

```
c
c VERSION : 900731
```

```
c
c PURPOSE : IRMA, substitute experimental NOE intensities in the theoretical
c NOE matrix
```

```
c
c CALL : MXMIX
```

```
c
c REFER. : -
```

```
c
c AUTHOR : Alexandre Bonvin
c Laboratory of Organic Chemistry
c Padualaan 8 , 3584 CH Utrecht, The Netherlands
```

```
c
c DESCRIPTION
```

```
c -----
```

```

c FILES   :
c
c   unit 1 : scaling factor
c
c   unit 2 : experimental NOE matrix
c
c   unit 3 : theoretical NOE matrix
c
c   unit 5 : standard input file with parameters for the calculations
c
c   unit 4 : output mixed matrix
c
c   unit 6 : standard output file
c
c PARAMETERS :
c
c ALGORITHM :
c
c USE       : subroutines
c
c   READNO (read input file)
c   SMKPOI (make pointer list and find matrix dimension)
c   SRDMX  (read a real*8 matrix)
c   SWRMX  (write a real*8 matrix)
c
c EXAMPLE   :
c
c=====

```

## 15.5.10 MXANNO

```

c=====
c
c PROGRAM : MXANNO
c -----
c VALID   : IRMA2
c
c VERSION : 900731
c
c PURPOSE : IRMA calculation of the relaxation matrix from the diagonalised
c           NOE matrix
c
c CALL    : MXANNO
c
c REFER.  : -
c
c   OLEJNICZAK, E.T., GAMPE, R.T.,JR. AND FESIK, S.W. (1986),
c       J. MAGN. RESON. 67, 28-41
c   MASSEFSKI, W.,JR. AND BOLTON, P.H. (1985),
c       J. MAGN. RESON. 65, 526-530
c   KEEPERS, J.W. AND JAMES, T.L. (1984), J. MAGN. RESON. 57, 404
c   MACURA, S., HUANG, Y., SUTER, D. AND ERNST, R.R. (1981),
c       J. MAGN. RESON. 43, 259-281
c   JEENER, J., MEIER, B.H., BACHMANN, P. AND ERNST, R.R. (1979)
c       J. CHEM. PHYS. 71, 4546

```

```

c SOLOMON, I. (1953), PHYS. REV. 99, 559-565
c
c AUTHOR : Alexandre Bonvin
c Laboratory of Organic Chemistry
c Padualaan 8 , 3584 CH Utrecht, The Netherlands
c
c
c DESCRIPTION
c -----
c FILES :
c
c unit 11... : input files containing the eigenvalues and
c eigenvectors
c
c unit 5 : standard input file
c
c unit 41... : output files for the relaxation matrices
c
c PARAMETERS : MAINDM is given in NOERE.INC
c
c ALGORITHM :
c
c USE : subroutines
c
c READNO (read input file)
c SMKPOI (make pointer list and find matrix dimension)
c SWRMX (write a real*8 matrix)
c
c EXAMPLE :
c
c=====

```

### 15.5.11 MXMER2

```

c=====
c
c PROGRAM : MXMER2
c -----
c VALID : IRMA2
c
c VERSION : 900801
c
c PURPOSE : IRMA averaging of the theoretical relaxation matrices
c
c CALL : MXMER2
c
c REFER. : -
c
c AUTHOR : Alexandre Bonvin
c Laboratory of Organic Chemistry
c Padualaan 8 , 3584 CH Utrecht, The Netherlands
c
c
c DESCRIPTION
c -----

```

```

c This program reads the relaxation matrices and puts them together to
c one by averaging and weighing them.
c
c FILES :
c
c unit 5 : default input used in all programs
c unit 11...: theoretical relaxation matrices, which have to be
c averaged
c unit 41...: experimental noe matrices, used for scaling
c
c
c unit 2 : average relaxation matrix
c unit 3 : upper bounds relaxation matrix
c unit 4 : lower bounds relaxation matrix
c unit 6 : standard output
c
c PARAMETERS :
c
c ALGORITHM :
c
c USE : subroutines
c
c READNO (read the input file)
c SMKPOI (make pointer list and find matrix dimension)
c
c EXAMPLE :
c
c=====

```

## 15.5.12 MXABLD

```

c=====
c
c PROGRAM : MXABLD
c -----
c VALID : IRMA2
c
c VERSION : 900802
c
c PURPOSE : IRMA calculate a distance matrix from a relaxation matrix
c
c CALL : MXABLD
c
c REFER. :
c
c OLEJNICZAK, E.T., GAMPE, R.T.,JR. AND FESIK, S.W. (1986),
c J. MAGN. RESON. 67, 28-41
c MASSEFSKI, W.,JR. AND BOLTON, P.H. (1985),
c J. MAGN. RESON. 65, 526-530
c KEEPERS, J.W. AND JAMES, T.L. (1984), J. MAGN. RESON. 57, 404
c MACURA, S., HUANG, Y., SUTER, D. AND ERNST, R.R. (1981),
c J. MAGN. RESON. 43, 259-281
c JEENER, J., MEIER, B.H., BACHMANN, P. AND ERNST, R.R. (1979)
c J. CHEM. PHYS. 71, 4546
c SOLOMON, I. (1953), PHYS. REV. 99, 559-565

```

```

c
c AUTHOR : Alexandre Bonvin
c   Laboratory of Organic Chemistry
c   Padualaan 8 , 3584 CH Utrecht, The Netherlands
c
c
c DESCRIPTION
c -----
c FILES   :
c
c   unit 2 : input order parameters file
c   unit 3 : input relaxation matrix
c   unit 4 : input chemical shift file
c   unit 5 : standard input file
c
c   unit 1 : output distance matrix
c   unit 6 : standard output file
c
c PARAMETERS : all parameters in sec, hz, ppm and angstrom
c
c ALGORITHM :
c
c USE       : subroutines
c
c   READNO (read input file)
c   SMKPOI (make pointer list and find matrix dimension)
c   RDS2MX (read order parameters matrix)
c   RDSHFT (read chemical shift file)
c   SRDMX  (real a real*8 matrix)
c   SWRMX  (write a real*8 matrix)
c
c EXAMPLE   :
c
c=====

```

### 15.5.13 MXRDIS

```

c=====
c
c PROGRAM : MXRDIS
c -----
c VALID   : IRMA2
c
c VERSION : 900815
c
c PURPOSE : IRMA, read distances matrices and create a distance file
c
c CALL    : MXRDIS
c
c REFER.  : -
c
c AUTHOR  : Alexandre Bonvin
c   Laboratory of Organic Chemistry
c   Padualaan 8 , 3584 CH Utrecht, The Netherlands
c

```

```

c
c DESCRIPTION
c -----
c FILES   :
c   unit 1 : upper distances matrix
c   unit 2 : distances matrix
c   unit 3 : lower distances matrix
c   unit 5 : standard input file with parameters for the calculations
c
c   unit 4 : output distances list
c   unit 6 : standard output file
c
c PARAMETERS :
c
c ALGORITHM :
c
c USE       : subroutines
c
c   READNO (read input file)
c   SMKPOI (make pointer list and find matrix dimension)
c   SRDMX  (read a real*8 matrix)
c
c EXAMPLE   :
c
c=====

```

### 15.3.14 MXRFAC

```

c=====
c
c PROGRAM : mxrfac
c -----
c VALID   : IRMA2
c
c VERSION : 900815
c
c PURPOSE : IRMA, read theoretical. matrices and calculate R-factors
c
c CALL    : mxrfac
c
c REFER.  : -
c
c AUTHOR  : Alexandre Bonvin
c           Laboratory of Organic Chemistry
c           Padualaan 8 , 3584 CH Utrecht, The Netherlands
c
c
c DESCRIPTION
c -----
c FILES   :
c   unit 11... : theoretical NOE matrices
c   unit 41... : experimental NOE matrices
c   unit 1     : standard input file with parameters for the calculations
c
c   unit 3     : output R-factor list

```

```

c      unit 6 : standard output file
c
c PARAMETERS :
c
c ALGORITHM :
c
c USE      : subroutines
c
c      READNO (read input file)
c      SMKPOI (make pointer list and find matrix dimension)
c      SRDMX  (read a real*8 matrix)
c
c EXAMPLE  :
c
c=====

```

### 15.5.15 MXSPC2

```

c=====
c
c PROGRAM : MXSPC2
c -----
c VALID   : IRMA2, 3D NMR
c
c VERSION : 900802
c
c PURPOSE : IRMA  mxspc2 calculates a 2d spectrum from a 2d matrix
c            of intensities at (i,j) + a list of chemical
c            shifts for each spin i or from a relaxation matrix.
c
c CALL    : MXSPC2
c
c REFER.  : -
c
c AUTHORS : Rolf Boelens and Alexandre Bonvin
c           Laboratory of Organic Chemistry
c           Padualaan 8 , 3584 CH Utrecht, The Netherlands
c
c
c DESCRIPTION
c -----
c FILES   : all files are requested by the program
c
c PARAMETERS : maximal dimension given by MAINDM in NOERE.INC
c
c ALGORITHM :
c
c USE      : subroutines
c
c      READNO (read input file)
c      SMKPOI (make pointer list and find matrix dimension)
c      SRDSHFT (read chemical shift file)
c      TEXTIN
c      RVALIN
c      IVALIN

```

c SRDMX (read a real\*8 matrix)

c

c EXAMPLE :

c

c=====

## 15.5.16 CONVER

c=====

c

c PROGRAM : CONVER

c -----

c VALID : IRMA2, GROMOS

c

c VERSION : 900802

c

c PURPOSE : IRMA generate all apolar protons and extract them from  
c GROMOS trajectory or coordinates files

c

c CALL : CONVER

c

c REFER. : -

c

c AUTHOR : Alexandre Bonvin

c Laboratory of Organic Chemistry

c Padualaan 8 , 3584 CH Utrecht, The Netherlands

c

c

c DESCRIPTION

c -----

c FILES :

c

c unit 4 : input file (see subroutine readgr)

c unit 10 : molecular topology file

c unit 11...: coordinates files or trajectory files (gromos)

c

c unit 1 : protons coordinates output file containing:

c

c line 1 ..... title

c line 2 ..... number of records (structures)

c line 3 ..... number of hydrogens per structure

c line 4 ..... x(1),y(1),z(1).....x(nhtot),y(nhtot),z(nhtot)

c for structure 1

c line n+4 .... x(1),y(1),z(1).....x(nhtot),y(nhtot),z(nhtot)

c for structure n

c

c unit 2 : all protons file in GROMOS format, the coordinates

c are from the first structure read. Only the protons

c names and numbers and residues names and number will

c be used in the IRMA in MKNOFL

c

c

c PARAMETERS : defined in NOERE.INC

c

c ALGORITHM :

```

c
c USE      : subroutines
c          READGR (read input file)
c          IXH   (generate all apolar protons)
c          EXTHH (extract the protons from the all atoms
c                coordinates)
c
c EXAMPLE  :
c
c=====
c-----
c
c  subroutine readgr(igrinp,nrfl,nris,nrrc,nskp,nrr,ntpi,npfi,
c +  npm,nrpi,ntb,niat,iacht,nforout)
c-----
c
c  this subroutine reads from tape(igrinp)the input parameters
c  used to read the gromos trajectory files and generate the
c  hydrogen atoms.
c
c  tape(igrinp):
c  -(7i10)
c  nrfl = number of files tape11-40 containing coordinates or
c         subaverages (.le.30)
c  nris = number of records to be skipped after reading the first
c         (title) record (ntr=1,ntpi<3)
c  nrrc = number of records per file to be read, after having read
c         the title record and nris coordinate records
c         (ntr=1,ntpi<3)
c  nskp : from every nskp records that are read, only the first one
c         is used, the last (nskp-1) ones are skipped, when
c         averaging (ntr=1,ntpi<3)
c  nrr = number of coordinates per record (.le.maxnrr-60,ntpi<3)
c  ntp = -1: input coordinates and title are read from normal
c         gromos coordinates files
c         = 0 : input coordinates and title record are unformatted
c         = 1 : input coordinates have been packed (ntr=1)
c         (see subr. pack), title record is unformatted
c         = 2 : input coordinates are formatted (ntr=1)
c         (see subr. pack), title record is formatted
c         = 3 : input coordinates are in standard formatted form
c         (nris=0,nrrc=1,nskp=1,nrr= not used)
c  npfi = number of digits behind decimal point of packed input
c         coordinates (ntpi=1)
c  -(3i10)
c  npm = sequence number of the molecule to be analysed
c  nrpi = number of solute atoms (including ions) per solute
c         molecule on tape11-40 (.ge. nrp from molecular topology)
c  ntb = 0 : no box
c         = 2 : solute in a box, box coordinates read from the
c         trajectory files
c  -(i10)
c  niat : number of integer atom codes that will be read below
c         for each of the four different geometries
c  -(8i10)
c  iacht(1...niat,1...4) : integer atom codes of the atoms that are
c         bound to the hydrogens atoms, for the four different

```

```

c      geometries. if an iac occurs more than once, only the
c      first occurrence will be used.
c
c      -(i10)
c      nforout = 0 proton coordinates trajectory file is formatted
c      = 1 proton coordinates trajectory file is unformatted
c      must be used when preparing file for IRMA
c
c=====

```

## 15.5.17 NOERELIB

```

C=====
C
C NOERE LIBRARY
C
C Alexandre Bonvin, Utrecht 900831
C
C This library contains the subroutines used in the
C IRMA2 programs.
C The following subroutines are included in this library:
C
C -SRDMX (read a real*8 matrix)
C -SWRMX (write a real*8 matrix)
C -SSCALT (scaling factor for theor. vs. exper. NOE matrices)
C -SCOREXP (correct experimental intensities)
C -SRCORR (correct theoretical intensities)
C -RDSHFT (read chemical shift file)
C -READNO (read input file)
C -SRDH (read and average coordinates file)
C -RDALLH (RDALLH2) (read a GROMOS coordinate file)
C -RDRESN (read a BUILDMAN result file)
C -SMKPOI (make a pointer list and find matrix dimension)
C -SRMATAV (create the relaxation matrix from coordinates)
C -DIS3 and DIS6 (functions calculating 1/dis**3 and 1/dis**6
C from coordinates)
C -SRMATAVD(create the relaxation matrix from distance matrix)
C -CHKTYP (check atom types, find methyl and aromatic protons)
C -RDS2MX (read order parameters matrix)
C -DIAGIV (diagonalisation subroutine)
C -GIVEIS
C -IMTQLV
C -TINVTB
C -TQL2
C -TRBK3B
C -TRED3B
C -GIVDIA
C -DIAHOU
C -DAXPY
C=====

```

## 15.6 Examples

This chapter contains examples of important files in IRMA2 and of command files.

### 15.6.1 IRMA2 input file

```
input IRMA test4
5.000E+08 Spectrometer frequency (Hz)
3.000E-09 Correlation time (s)
0.80000 Additional leakage rate for the diagonal (s-1)
1.58464 1.000E-10 Extra diag. relaxation contribution and correlation time for methyls
10.00000 Scaling factor for the coordinates (--> Å)
1.00000 1.00000 Standard deviation factors
F Chemical shift is included (T/F)
T Order parameters are included (T) or not (F)
T T T Matrix form : EXP, THEO, S**2 (form(T) or unform(F))
1 0=no 1=yes symmetrize exp. NOE matrices
-1 exp.NOEs: skip neg.(-1),skip pos.(1), noskip (0)
0 Type of averaging 0=int. 1=tm 2=none
T skip unassigned stereo. H (T/F)
6 distances averaging 6=<1/r**6> 3=<1/r**3>
1 Reference peaks
6 5 1TYR H CB2 1TYR H CB1
3 1 averaging type for methyl and aromatic groups
18 Total number of protons
0 0 1 1 0 0 0 0 0 1 TYR H1 1
0 0 1 2 0 0 0 0 0 1 TYR H2 2
0 0 1 3 0 0 0 0 0 1 TYR H3 4
0 0 1 4 0 0 0 0 0 1 TYR H CA1 6
0 0 1 5 0 0 0 0 0 1 TYR H CB1 8
0 0 1 6 0 0 0 0 0 1 TYR H CB2 9
2 0 2 7 8 9 0 0 0 1 TYR HCD11 12
1 1 1 8 0 0 0 0 0 1 TYR HCD21 14
2 0 2 9 10 7 0 0 0 1 TYR HCE11 16
1 1 1 10 0 0 0 0 0 1 TYR HCE21 18
0 0 1 11 0 0 0 0 0 1 TYR HH 21
0 0 1 12 0 0 0 0 0 2 THR H 22
0 0 1 13 0 0 0 0 0 2 THR H CA1 27
0 0 1 14 0 0 0 0 0 2 THR H CB1 29
0 0 1 15 0 0 0 0 0 2 THR HG1 31
3 0 3 16 17 18 0 0 0 2 THR HCG21 33
3 2 2 17 18 0 0 0 0 2 THR HCG22 34
3 2 1 18 0 0 0 0 0 2 THR HCG23 35
6 Number of mixing times
0.02000 0.04000 0.08000 0.12000 0.16000 0.25000
11 Number of NOEs constraints
4 5 2.460E+06 4.460E+06 6.280E+06 9.690E+06 1.160E+07 1.460E+07
4 6 2.380E+06 4.410E+06 4.670E+06 7.060E+06 9.260E+06 1.200E+07
5 4 4.620E+06 5.860E+06 8.180E+06 1.340E+07 1.440E+07 1.870E+07
6 5 2.640E+07 4.900E+07 6.190E+07 7.080E+07 7.310E+07 7.780E+07
6 4 3.280E+06 3.190E+06 5.520E+06 7.150E+06 1.010E+07 1.280E+07
7 9 2.215E+07 2.134E+07 3.117E+07 2.728E+07 3.713E+07 4.636E+07
4 7 -6.667E+05 6.441E+05 1.491E+06 2.728E+06 3.405E+06 3.774E+06
5 7 7.507E+05 2.112E+05 3.467E+05 1.690E+06 1.255E+06 3.343E+06
6 12 3.794E+05 6.748E+05 9.619E+05 1.775E+06 2.277E+06 2.830E+06
```

```

5 12 3.692E+05 1.858E+05 8.697E+05 9.353E+05 1.820E+06 1.995E+06
16 12 9.045E+05 1.676E+06 3.261E+06 5.743E+06 7.898E+06 1.005E+07

```

### 15.6.2 Proton coordinates file

THIS IS A TEST FILE WITH A PART OF A PROTEIN

```

18
1TYR   H1   1  0.161  1.329  0.565
1TYR   H2   2  0.111  1.313  0.565
1TYR   H3   4  0.210  1.329  0.565
1TYR  H CA1  6 -0.027  1.238  0.683
1TYR  H CB1  8  0.054  1.189  0.451
1TYR  H CB2  9  0.176  1.080  0.521
1TYR HCD11 12 -0.193  1.140  0.576
1TYR HCD21 14  0.121  0.854  0.489
1TYR HCE11 16 -0.360  0.954  0.587
1TYR HCE21 18 -0.048  0.668  0.497
1TYR   HH  21 -0.264  0.614  0.527
2THR   H  25  0.313  1.145  0.747
2THR  H CA1 27  0.211  0.935  0.919
2THR  H CB1 29  0.445  0.834  0.895
2THR  HG1  31  0.578  0.950  0.727
2THR HCG21 33  0.426  0.758  0.675
2THR HCG22 34  0.259  0.791  0.729
2THR HCG23 35  0.342  0.906  0.621

```

### 15.6.3 IRMA2 distance output file

```

IRMA distances
11
1 TYR  H CA1  6  1 TYR  H CB1  8  2.691  2.591  2.512
1 TYR  H CA1  6  1 TYR  H CB2  9  3.070  3.004  2.946
1 TYR  H CB1  8  1 TYR  H CA1  6  2.691  2.591  2.512
1 TYR  H CB2  9  1 TYR  H CB1  8  1.837  1.804  1.775
1 TYR  H CB2  9  1 TYR  H CA1  6  3.070  3.004  2.946
1 TYR HCD11 12  1 TYR HCE11 16  3.002  2.833  2.714
1 TYR  H CA1  6  1 TYR HCD11 12  4.294  4.144  4.025
1 TYR  H CB1  8  1 TYR HCD11 12 999.000  0.000  0.000
1 TYR  H CB2  9  2 THR   H  25  4.187  4.125  4.070
1 TYR  H CB1  8  2 THR   H  25  4.341  4.093  3.919
2 THR HCG21 33  2 THR   H  25  4.652  4.596  4.544

```

### 15.6.4 Thenoes.job (VAX/VMS)

```

$ ! CALCULATION OF THEORETICAL NOES ON BASIS OF A MODEL
$ SET DEFAULT $DISK3:[MANUEL.IRMA2.TEST4]
$ ASS/USER TEST4.MDH FOR001
$ ASS/USER TEST4.ORD FOR002

```

```

$ ASS/USER MXTEST4 FOR003
$ ASS/USER TEST4.SHIFT FOR004
$ ASS/USER TEST4.INP FOR005
$ RUN $DISK3:[MANUEL.IRMA2.PRGRMS]MXBLD
$ ASS/USER MXTEST4 FOR003
$ ASS/USER EIGTEST4 FOR002
$ ASS/USER TEST4.INP FOR005
$ RUN $DISK3:[MANUEL.IRMA2.PRGRMS]MXGEIS
$ DEL/NOCON MXTEST4.DAT;*
$ NUM=1
$ LOOP:
$ ASS/USER NOESTEST4'NUM' FOR01'NUM'
$ NUM=NUM+1
$ IF NUM.LE.6 THEN GOTO LOOP
$ ASS/USER EIGTEST4 FOR003
$ ASS/USER TEST4.INP FOR005
$ RUN $DISK3:[MANUEL.IRMA2.PRGRMS]MX2DNO
$ DEL/NOCON EIGTEST4.DAT;*

```

### 15.6.5 Mxcrex.job (VAX/VMS)

```

$ ! CALCULATION OF EXPERIMENTAL NOES ON BASIS OF RESULT FILES
$ SET DEFAULT $DISK3:[MANUEL.IRMA2.TEST4]
$ ASS/USER TEST4.INP FOR005
$ NUM3=1
$ LOOP2:
$ CN=NUM3
$ ASS/USER EXPTEST4'NUM3' FOR04'NUM3'
$ NUM3=NUM3+1
$ IF CN .GE. 6 THEN GOTO CALC
$ GOTO LOOP2
$ CALC:
$ RUN $DISK3:[MANUEL.IRMA2.PRGRMS]MXCREX

```

### 15.6.6 Mergnoes.job (VAX/VMS)

```

$ ! MERGING OF BOTH NOE MATRICES AND DISTANCE CALCULATION
$ SET DEFAULT $DISK3:[MANUEL.IRMA2.TEST4]
$ NUM=1
$ LOOP:
$ ASS/USER NOESTEST4'NUM' FOR01'NUM'
$ ASS/USER EXPTEST4'NUM' FOR04'NUM'
$ NUM=NUM+1
$ IF NUM .LE. 6 THEN GOTO LOOP
$ ASS/USER TEST4.INP FOR005
$ ASS/USER SCALTEST4 FOR001
$ RUN $DISK3:[MANUEL.IRMA2.PRGRMS]MXSCAL
$ NUM=1
$ LOOP2:
$ ASS/USER TEST4.INP FOR005
$ ASS/USER NOESTEST4'NUM' FOR003
$ ASS/USER EXPTEST4'NUM' FOR002
$ ASS/USER MATOUTTEST4'NUM' FOR004
$ ASS/USER SCALTEST4 FOR001

```

```

$ RUN $DISK3:[MANUEL.IRMA2.PRGRMS]MXMIX
$ ASS/USER TEST4.INP FOR005
$ ASS/USER MATOUTTEST4'NUM' FOR003
$ ASS/USER ANEIGTEST4'NUM' FOR002
$ RUN $DISK2:[MANUEL.IRMA2.PRGRMS]MXGEIS
$ DEL/NOCON MATOUTTEST4'NUM'.DAT;*
$ NUM=NUM+1
$ IF NUM .LE. 6 THEN GOTO LOOP2
$ NUM=1
$ LOOP3:
$ ASS/USER ANEIGTEST4'NUM' FOR01'NUM'
$ ASS/USER ANMXTEST4'NUM' FOR04'NUM'
$ NUM=NUM+1
$ IF NUM .LE. 6 THEN GOTO LOOP3
$ ASS/USER TEST4.INP FOR005
$ RUN $DISK3:[MANUEL.IRMA2.PRGRMS]MXANNO
$ DEL/NOCON ANEIGTEST4*.DAT;*
$ NUM=1
$ LOOP4:
$ ASS/USER ANMXTEST4'NUM' FOR01'NUM'
$ ASS/USER EXPTEST4'NUM' FOR04'NUM'
$ NUM=NUM+1
$ IF NUM .LE. 6 THEN GOTO LOOP4
$ ASS/USER TEST4.INP FOR005
$ ASS/USER ANMXNEWTEST4 FOR002
$ ASS/USER ANMXUPTTEST4 FOR003
$ ASS/USER ANMXLOTTEST4 FOR004
$ RUN $DISK3:[MANUEL.IRMA2.PRGRMS]MXMER2
$ ASS/USER TEST4.INP FOR005
$ ASS/USER ANMXNEWTEST4 FOR003
$ ASS/USER TEST4.ORD FOR002
$ ASS/USER TEST4.SHIFT FOR004
$ ASS/USER DISNEWTEST4 FOR001
$ RUN $DISK3:[MANUEL.IRMA2.PRGRMS]MXABLD
$ ASS/USER TEST4.INP FOR005
$ ASS/USER ANMXUPTTEST4 FOR003
$ ASS/USER TEST4.ORD FOR002
$ ASS/USER TEST4.SHIFT FOR004
$ ASS/USER DISUPTTEST4 FOR001
$ RUN $DISK3:[MANUEL.IRMA2.PRGRMS]MXABLD
$ ASS/USER TEST4.INP FOR005
$ ASS/USER ANMXLOTTEST4 FOR003
$ ASS/USER TEST4.ORD FOR002
$ ASS/USER TEST4.SHIFT FOR004
$ ASS/USER DISLOTTEST4 FOR001
$ RUN $DISK3:[MANUEL.IRMA2.PRGRMS]MXABLD
$ DEL/NOCON ANMX*.*;*

```

### 15.6.7 Thenoes.job (UNIX)

```

# ! CALCULATION OF THEORETICAL NOES ON BASIS OF A MODEL
ln -s test4.mdh fort.1
ln -s test4.ord fort.2
ln -s test4.shift fort.4

```

```

ln -s mxtest4 fort.3
/usr1/people/irma/irma2/prgrms/mxbld <test4.inp
/bin/rm fort.1
/bin/rm fort.2
/bin/rm fort.3
/bin/rm fort.4
#
ln -s mxtest4 fort.3
ln -s eigtest4 fort.2
/usr1/people/irma/irma2/prgrms/mxgeis <test4.inp
/bin/rm fort.2
/bin/rm fort.3
/bin/rm mxtest4
#
ln -s noestest41 fort.11
ln -s noestest42 fort.12
ln -s noestest43 fort.13
ln -s noestest44 fort.14
ln -s noestest45 fort.15
ln -s noestest46 fort.16
ln -s eigtest4 fort.3
/usr1/people/irma/irma2/prgrms/mx2dno <test4.inp
/bin/rm fort.11
/bin/rm fort.12
/bin/rm fort.13
/bin/rm fort.14
/bin/rm fort.15
/bin/rm fort.16
/bin/rm fort.3
/bin/rm eigtest4

```

### 15.6.8 Mxcrex.job (UNIX)

```

# ! CALCULATION OF EXPER. NOES ON BASIS OF RESULTFILES
ln -s exptest41 fort.41
ln -s exptest42 fort.42
ln -s exptest43 fort.43
ln -s exptest44 fort.44
ln -s exptest45 fort.45
ln -s exptest46 fort.46
/usr1/people/irma/irma2/prgrms/mxcrex <test4.inp
/bin/rm fort.41
/bin/rm fort.42
/bin/rm fort.43
/bin/rm fort.44
/bin/rm fort.45
/bin/rm fort.46

```

### 15.6.9 Mergnoes.job (UNIX)

```

# ! MERGING OF BOTH NOE MATRICES AND DISTANCE CALCULATION
#

```

```

ln -s noestest41 fort.11
ln -s exptest41 fort.41
ln -s noestest42 fort.12
ln -s exptest42 fort.42
ln -s noestest43 fort.13
ln -s exptest43 fort.43
ln -s noestest44 fort.14
ln -s exptest44 fort.44
ln -s noestest45 fort.15
ln -s exptest45 fort.45
ln -s noestest46 fort.16
ln -s exptest46 fort.46
ln -s scaltest4 fort.1
/usr1/people/irma/irma2/prgrms/mxscal <test4.inp
/bin/rm fort.11
/bin/rm fort.41
/bin/rm fort.12
/bin/rm fort.42
/bin/rm fort.13
/bin/rm fort.43
/bin/rm fort.14
/bin/rm fort.44
/bin/rm fort.15
/bin/rm fort.45
/bin/rm fort.16
/bin/rm fort.46
/bin/rm fort.1
#
ln -s noestest41 fort.3
ln -s exptest41 fort.2
ln -s matouttest41 fort.4
ln -s scaltest4 fort.1
/usr1/people/irma/irma2/prgrms/mxmix <test4.inp
/bin/rm fort.1
/bin/rm fort.2
/bin/rm fort.3
/bin/rm fort.4
ln -s matouttest41 fort.3
ln -s aneigtest41 fort.2
/usr1/people/irma/irma2/prgrms/mxgeis <test4.inp
/bin/rm fort.2
/bin/rm fort.3
/bin/rm matouttest41
ln -s noestest42 fort.3
ln -s exptest42 fort.2
ln -s matouttest42 fort.4
ln -s scaltest4 fort.1
/usr1/people/irma/irma2/prgrms/mxmix <test4.inp
/bin/rm fort.1
/bin/rm fort.2
/bin/rm fort.3
/bin/rm fort.4
ln -s matouttest42 fort.3
ln -s aneigtest42 fort.2
/usr1/people/irma/irma2/prgrms/mxgeis <test4.inp
/bin/rm fort.2
/bin/rm fort.3
/bin/rm matouttest42

```

```

ln -s noestest43 fort.3
ln -s exptest43 fort.2
ln -s matouttest43 fort.4
ln -s scaltest4 fort.1
/usr1/people/irma/irma2/prgrms/mxmix <test4.inp
/bin/rm fort.1
/bin/rm fort.2
/bin/rm fort.3
/bin/rm fort.4
ln -s matouttest43 fort.3
ln -s aneigtest43 fort.2
/usr1/people/irma/irma2/prgrms/mxgeis <test4.inp
/bin/rm fort.2
/bin/rm fort.3
/bin/rm matouttest43
ln -s noestest44 fort.3
ln -s exptest44 fort.2
ln -s matouttest44 fort.4
ln -s scaltest4 fort.1
/usr1/people/irma/irma2/prgrms/mxmix <test4.inp
/bin/rm fort.1
/bin/rm fort.2
/bin/rm fort.3
/bin/rm fort.4
ln -s matouttest44 fort.3
ln -s aneigtest44 fort.2
/usr1/people/irma/irma2/prgrms/mxgeis <test4.inp
/bin/rm fort.2
/bin/rm fort.3
/bin/rm matouttest44
ln -s noestest45 fort.3
ln -s exptest45 fort.2
ln -s matouttest45 fort.4
ln -s scaltest4 fort.1
/usr1/people/irma/irma2/prgrms/mxmix <test4.inp
/bin/rm fort.1
/bin/rm fort.2
/bin/rm fort.3
/bin/rm fort.4
ln -s matouttest45 fort.3
ln -s aneigtest45 fort.2
/usr1/people/irma/irma2/prgrms/mxgeis <test4.inp
/bin/rm fort.2
/bin/rm fort.3
/bin/rm matouttest45
ln -s noestest46 fort.3
ln -s exptest46 fort.2
ln -s matouttest46 fort.4
ln -s scaltest4 fort.1
/usr1/people/irma/irma2/prgrms/mxmix <test4.inp
/bin/rm fort.1
/bin/rm fort.2
/bin/rm fort.3
/bin/rm fort.4
ln -s matouttest46 fort.3
ln -s aneigtest46 fort.2
/usr1/people/irma/irma2/prgrms/mxgeis <test4.inp
/bin/rm fort.2

```

```

/bin/rm fort.3
/bin/rm matouttest46
#
ln -s aneigtest41 fort.11
ln -s anmxtest41 fort.41
ln -s aneigtest42 fort.12
ln -s anmxtest42 fort.42
ln -s aneigtest43 fort.13
ln -s anmxtest43 fort.43
ln -s aneigtest44 fort.14
ln -s anmxtest44 fort.44
ln -s aneigtest45 fort.15
ln -s anmxtest45 fort.45
ln -s aneigtest46 fort.16
ln -s anmxtest46 fort.46
/usr1/people/irma/irma2/prgrms/mxanno <test4.inp
/bin/rm fort.11
/bin/rm fort.41
/bin/rm aneigtest41
/bin/rm fort.12
/bin/rm fort.42
/bin/rm aneigtest42
/bin/rm fort.13
/bin/rm fort.43
/bin/rm aneigtest43
/bin/rm fort.14
/bin/rm fort.44
/bin/rm aneigtest44
/bin/rm fort.15
/bin/rm fort.45
/bin/rm aneigtest45
/bin/rm fort.16
/bin/rm fort.46
/bin/rm aneigtest46
#
ln -s anmxtest41 fort.11
ln -s exptest41 fort.41
ln -s anmxtest42 fort.12
ln -s exptest42 fort.42
ln -s anmxtest43 fort.13
ln -s exptest43 fort.43
ln -s anmxtest44 fort.14
ln -s exptest44 fort.44
ln -s anmxtest45 fort.15
ln -s exptest45 fort.45
ln -s anmxtest46 fort.16
ln -s exptest46 fort.46
ln -s anmxnewtest4 fort.2
ln -s anmxuptest4 fort.3
ln -s anmxlotest4 fort.4
/usr1/people/irma/irma2/prgrms/mxmer2 <test4.inp
/bin/rm fort.11
/bin/rm fort.41
/bin/rm anmxtest41
/bin/rm fort.12
/bin/rm fort.42
/bin/rm anmxtest42
/bin/rm fort.13

```

```

/bin/rm fort.43
/bin/rm anmxtest43
/bin/rm fort.14
/bin/rm fort.44
/bin/rm anmxtest44
/bin/rm fort.15
/bin/rm fort.45
/bin/rm anmxtest45
/bin/rm fort.16
/bin/rm fort.46
/bin/rm anmxtest46
/bin/rm fort.2
/bin/rm fort.3
/bin/rm fort.4
#
ln -s anmxnewtest4 fort.3
ln -s test4.ord      fort.2
ln -s test4.shift   fort.4
ln -s disnewtest4  fort.1
/usr1/people/irma/irma2/prgrms/mxabld <test4.inp
/bin/rm fort.1
/bin/rm fort.2
/bin/rm fort.3
/bin/rm fort.4
/bin/rm anmxnewtest4
#
ln -s anmxuptest4 fort.3
ln -s test4.ord      fort.2
ln -s test4.shift   fort.4
ln -s disuptest4  fort.1
/usr1/people/irma/irma2/prgrms/mxabld <test4.inp
/bin/rm fort.1
/bin/rm fort.2
/bin/rm fort.3
/bin/rm fort.4
/bin/rm anmxuptest4
#
ln -s anmxlotest4 fort.3
ln -s test4.ord      fort.2
ln -s test4.shift   fort.4
ln -s dislotest4  fort.1
/usr1/people/irma/irma2/prgrms/mxabld <test4.inp
/bin/rm fort.1
/bin/rm fort.2
/bin/rm fort.3
/bin/rm fort.4
/bin/rm anmxlotest4

```

## 15.7 References

- 1 R. Boelens, T.M.G. Koning and R. Kaptein (1988), *J. Mol. Struc.* 173, 299
- 2 R. Boelens, T.M.G. Koning, G.A. van der Marel, J.H. van Boom and R. Kaptein (1989), *J. Magn. Res.* 82, 290
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