

## README for the JCAMP-DX nD-NMR test file round robin.

### 1) In JCAMP-DX 6.0 for 2D-NMR there are three new labels:

- **##NUM\_DIM= 2**  
Provides the dimensionality of the data set.
- **##.ACQUISITION SCHEME= NOT PHASE SENSITIVE**  
In two dimensional data sets a new DATA TABLE belonging to the second independent variable T1 or F1 exists. These DATA TABLES can only be assigned to the T1 values when the acquisition method (phase sensitive, not phase sensitive) is known. By phase sensitive data the data acquisition technique (STATES, TPPI, TPPI-STATES) must also be described, as the T1-data is stored differently in the three methods.
- **##.NUCLEUS= 1H, 13C**  
Defined as the nucleus for the particular axis.

### 2) The following labels arose out of the Version 5.01 publication which is currently submitted for publication:

- **##.SOLVENT NAME=**  
Solvent
- **##.PULSE SEQUENCE= HETCOR**  
Pulse Sequence in the newly defined format. The definition is restricted to the most popular pulse sequences and is not a generic method for defining pulse sequences.
- **##UNITS= ... POWER**  
New YUNITS for Power spectra

### 3) The following labels are used differently to the description in JCAMP-DX 5.00:

example ATTRIBUTE TABLES

```
##NTUPLES= nD NMR FID
##VAR_NAME= TIME1,          TIME2,          FID/REAL,          FID/IMAG
##SYMBOL=   T1,            T2,            R,                I
##.NUCLEUS= NUCLEUS_T1,    NUCLEUS_T2
##VAR_TYPE= INDEPENDENT,   INDEPENDENT,    DEPENDENT,        DEPENDENT
##VAR_FORM= AFFN,          ASDF,           ASDF,             ASDF
##VAR_DIM=  VAR_DIM_T1,    VAR_DIM_T2,     VAR_DIM_R,        VAR_DIM_I
##UNITS=     SECONDS,      SECONDS,        ARBITRARY UNITS,  ARBITRARY UNITS
##FIRST=     FIRST_T1,     FIRST_T2, ,    $$FIRST_R and FIRST_I are in the Pages
##LAST=      LAST_T1,     LAST_T2, ,
##MIN=       MIN_T1,      MIN_T2,          MIN_R,            MIN_I
##MAX=       MAX_T1,      MAX_T2,          MAX_R,            MAX_I
##FACTOR=    FACTOR_T1,   FACTOR_T2,       FACTOR_R,         FACTOR_I

##NTUPLES= nD NMR SPECTRUM
##VAR_NAME= FREQUENCY1,    FREQUENCY2,      SPECTRUM
##SYMBOL=   F1,            F2,              Y
##.NUCLEUS= NUCLEUS_F1,    NUCLEUS_F2
##VAR_TYPE= INDEPENDENT,   INDEPENDENT,     DEPENDENT
##VAR_FORM= AFFN,          ASDF,             ASDF
##VAR_DIM=  VAR_DIM_F1,    VAR_DIM_F2,       VAR_DIM_Y
##UNITS=     HZ,           HZ,               POWER
##FIRST=     FIRST_F1,     FIRST_F2,          $$FIRST_Y is in the Pages
##LAST=      LAST_F1,     LAST_F2,
##MIN=       MIN_F1,      MIN_F2,           MIN_Y
##MAX=       MAX_F1,      MAX_F2,           MAX_Y
##FACTOR=    FACTOR_F1,   FACTOR_F2,        FACTOR_Y
```

- An extra independent variable, T1 for FIDs and F1 for spectra is available for the second axis of the data set. This extra variable requires an extra column in the "ATTRIBUTE TABLE". As the second independent variable can be used to differentiate the PAGES the PAGE NUMBER N used in JCAMP-DX 5.00 is no longer necessary.

- **##PAGE= T1= 0.1144165E-03 (for FIDs or )**  
**##PAGE= F1= 4370.000 (for spectra)**

The actual value of the second independent variable is given as an argument in each PAGE.

- **##FIRST= 0.1144165E-03, 0.00, 13165, 2733**

The first Y-value (or for FIDs the first value of R and I) is different for each PAGE. It is therefore not possible to provide them in the ATTRIBUTE TABLE. For this reason each PAGE contains it's own FIRST LDR.

In the ATTRIBUTE TABLE are only the FIRST and LAST for T1 and T2 (for FIDs) or F1 and F2 (for spectra) provided to enable the calculation of the increment in the independent variables analogue to the formula  $(LASTX - FIRSTX) / (NPOINTS - 1)$ .

The parameter SW is redundant in both dimensions as SW can be calculated from VAR\_DIM, LAST and FIRST:

$SW2 = (VAR\_DIM\_T2 - 1) / (LAST\_T2 - FIRST\_T2)$  and

$SW1 = (VAR\_DIM\_T1 - 1) / (n * (LAST\_T1 - FIRST\_T1))$ ,

where n=1 or 2, depending on the pulse experiment.

- **##DATA TABLE= (T2++(R..R)), PROFILE**

The variable X from JCAMP-DX 5.00 is replaced by T2 or F2.