Bayesian Analysis Users Guide
Release 4.00, Manual Version 1

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Chapter 14

Magnetization Transfer

The Magnetization transfer package analyzes two site magnetization exchange data. This data is obtained from a peak pick, a Bayes Analyze file or it can be manually entered and loaded as an Ascii file. The Ascii data used in this package are generated from an Fid. The Fid data should be an arrayed inversion recovery data set. If we call the two sites that are exchanging magnetization Site A, and Site B, then the data should be in inversion recover data set where Site A was inverted. You should also have a data set where Site B was inverted. Finally, you can also invert both sites and that data may also be used. Preferably, you should array these Fid so as to obtain as many data values as possible on each recovery curve, the more data you have the more precise you parameter estimates will be. Note, that while it is not recommended, a single inversion recover data set can be used and you will be able to get exchange rates. However, because of the limited about of data, they will probably be highly uncertain. The interface to this package is shown in Fig. 14.1. To use this package, you must do the following:

Select the Magnetization Transfer package from the Package menu.

Load at lease one and preferably two three column Ascii data sets using the Files menu. The three columns are the abscissa value, and the amplitude or peak value of the Site A and B magnetization. Additionally, you can load an arrayed Fid and then use a double cursor to mark the center of the two exchanging peaks and use the "Get Peak" button on the bottom right of the Fid viewer. When a data set has been successfully loaded a plot contain the two sites is displayed in the Ascii Data viewer. For Fids, to load a second peak pick or Bayes Analyze file, simply load a second Fid and either load a peak pick or a Bayes Analyze file. Finally, if you have analyzed this Fid using Bayes Analyze you can load the resonance amplitude from the Bayes Analyze files using the "Files/Load Bayes Analyze" menu.

Check the Analysis Options/Find Outliers box if you suspect outliers are present in the data.

Normally the prior probabilities for the parameters would normally have to be reviewed here. However, the calculations are done using a variable transformation, sum and difference variables and this change of variables makes determining prior ranges so easy that the package does it automatically.

Select the server that is to process the analysis.

Figure 14.1: The Magnetization Transfer Package Interface

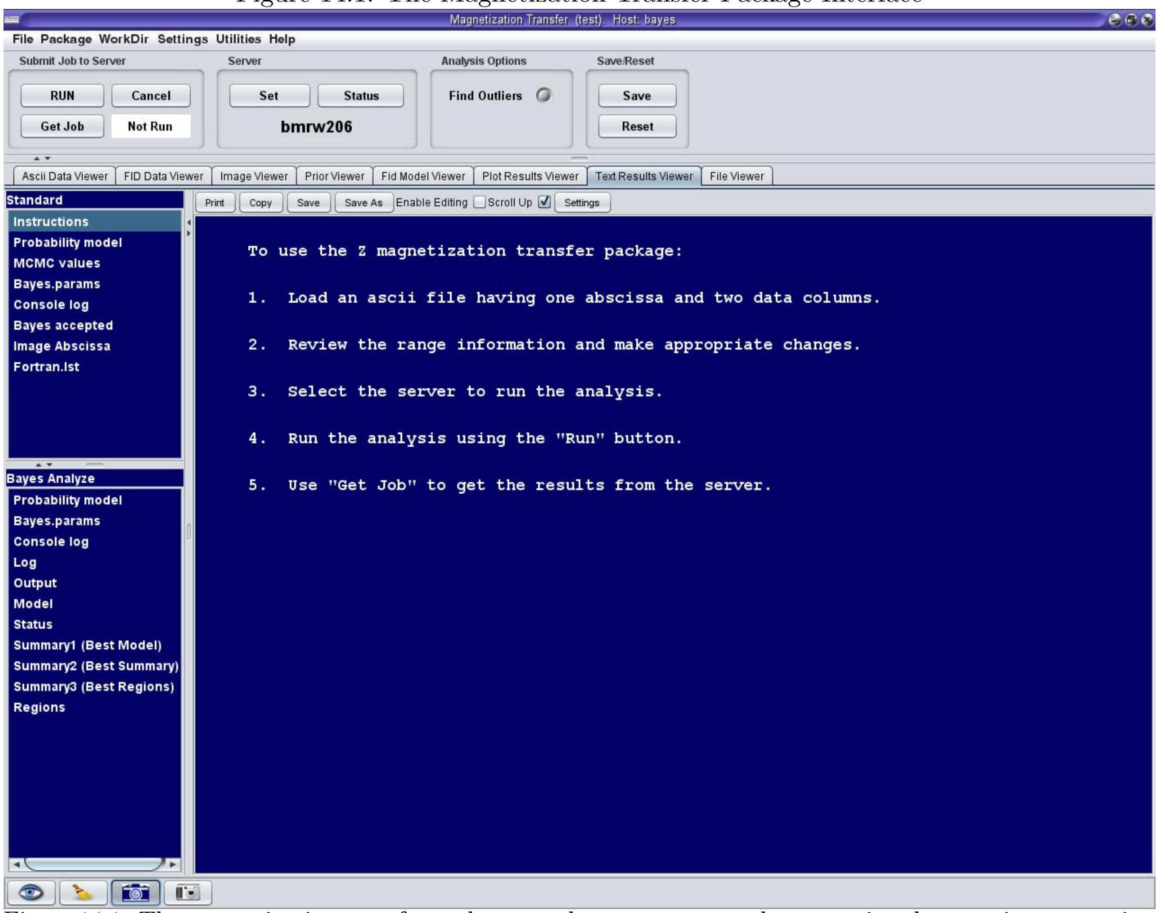

Figure 14.1: The magnetization transfer packages analyzes one or more data set using the equations governing two site magnetization exchange. The inferred parameters are the two exchange rates and the two relaxation rates. For more on the actual calculations and the widgets see the text.

Check the status of the selected server to determine if the server is busy, change to another server if the selected server is busy.

Run the the analysis on the selected server by activating the Run button.

Get the the results of the analysis by activating the Get Job button. If the analysis is running, this button will return the Accepted report containing the status of the current run. Otherwise, it will fetch and display the results from the current analysis.

14.1 The Bayesian Calculation

The two site magnetization transfer package solves problems involving magnetization transfer. If we designate the two sites as "a" and "b" respectively then the magnetization transfer model of the "a" site is related to the data by

$$d_a(t_i) = M_a(t_i) + \text{error} \tag{14.1}$$

and similarly for the "b" site,

$$d_b(t_i) = M_b(t_i) + \text{error} \tag{14.2}$$

where $M_a(t)$ and $M_b(t)$ are the solution to the Block-McConnell equations, and "error" represents noise in the data and should not be taken to mean that this noise is the same in both data sets. McConnell's modification to the Block equation is given by

$$\frac{dM_a(t)}{dt} = -R_{1a}[M_a(t) - M_a(\infty)] - K_{ab}M_a(t) + K_{ba}M_b(t) \tag{14.3}$$

$$\frac{dM_b(t)}{dt} = -R_{1b}[M_b(t) - M_b(\infty)] - K_{ba}M_b(t) + K_{ab}M_a(t) \tag{14.4}$$

where R_{1a} and R_{1b} are the relaxation rates for the "a" and "b" sites, K_{ba} is the rate at which magnetization goes from the "b" to the "a" site. Similarly K_{ab} is the rate at which magnetization exchanges from the "a" to the "b" site.

These equations are coupled linear first order differential equations and their bi-exponential solution is given by

$$M_a(t) = H(t)M_a(0) + G(t)M_b(0) + \left[1 - H(t) - G(t)\frac{K_{ab}}{K_{ba}}\right] M_a(\infty) \tag{14.5}$$

$$M_b(t) = I(t)M_b(0) - J(t)M_a(0) + \left[J(t) + [1 - I(t)]\frac{K_{ba}}{K_{ba}}\right] M_a(\infty) \tag{14.6}$$

where $M_a(\infty)$ is the equilibrium magnetization for the "a" site, and $M_a(0)$ and $M_b(0)$ are the initial magnetization for the "a" and "b" sites. The functions $G(t)$, $H(t)$, $I(t)$ and $J(t)$ are defined as

$$G(t) = \frac{\exp\{\alpha_1 t\} - \exp\{\alpha_2 t\}}{U - V}, \tag{14.7}$$

$$H(t) = \frac{U\exp\{\alpha_2 t\} - V\exp\{\alpha_1 t\}}{U - V}, \tag{14.8}$$

$$I(t) = \frac{U\exp\{\alpha_1 t\} - V\exp\{\alpha_2 t\}}{U - V}, \tag{14.9}$$

$$J(t) = UVG(t), \tag{14.10}$$

with

$$U = \frac{\alpha_1 + K_{ab} + R_{1a}}{K_{ba}}, \tag{14.11}$$

$$V = \frac{\alpha_2 + K_{ab} + R_{1a}}{K_{ba}}. \tag{14.12}$$

The observed decay rates α_1 and α_2 are given by

$$\alpha_{1,2} = -\frac{R_{1a} + R_{1b} + K_{ab} + K_{ba}}{2} \pm \frac{1}{2}\sqrt{(R_{1a} - R_{1b} - K_{ab} - K_{ba})^2 + 4K_{ab}K_{ba}} \tag{14.13}$$

where α_1 takes the plus and α_2 the minus.

The four parameters of interest are the two exchange rates K_{ab} and K_{ba} and the two relaxation rates R_{1a} and R_{1b}. In addition there are three parameters per "a" and "b" site that must be included, two initial conditions magnetizations, $M_a(0)$ and $M_b(0)$ and one equilibrium magnetization $M_a(\infty)$. The equilibrium condition,

$$M_b(\infty) = M_a(\infty)\frac{K_{ab}}{K_{ba}} \tag{14.14}$$

was used to eliminate $M_b(\infty)$.

Before we start the process of computing the posterior probability for the parameters of interest, K_{ab}, K_{ba}, R_{1a} and R_{1b}, we are going to rewrite the model equations and the data into a form that is more convenient for the upcoming analytic calculation. First we are going to define a single data set D with data item $d(t_i)$ that is the "a" site data followed by the "b" site data:

$$d(t_i) = \begin{cases} d_a(t_i) & \text{if } 1 \le i \le N \\ d_b(t_j) & \text{if } 1 \le j \le N \text{ with } j \equiv i - N \end{cases} \tag{14.15}$$

where the index i ranges from 1 up to $2N$. This definition is roughly like defining a complex data set with the "a" site being the real data and the "b" site being the imaginary data. Next we will rewrite Eqs. (14.1 and 14.2) into a single equation:

$$d(t_i) = \sum_{k=1}^{3} M_k \mathcal{H}_k(t_i) + \text{error} \tag{14.16}$$

where $M_1 \equiv M_a(0)$, $M_2 \equiv M_b(0)$ and $M_3 \equiv M_a(\infty)$. Finally, the three functions $\mathcal{H}_1(t_i)$, $\mathcal{H}_2(t_i)$ and $\mathcal{H}_3(t_i)$ are defined as

$$\mathcal{H}_1(t_i) = \begin{cases} H(t_i) & \text{if } 1 \le i \le N \\ -J(t_j) & \text{if } 1 \le j \le N \text{ with } j \equiv i - N \end{cases}, \tag{14.17}$$

$$\mathcal{H}_2(t_i) = \begin{cases} G(t_i) & \text{if } 1 \le i \le N \\ I(t_j) & \text{if } 1 \le j \le N \text{ with } j \equiv i - N \end{cases} \tag{14.18}$$

and

$$\mathcal{H}_3(t_i) = \begin{cases} (1 - H(t_i) - G(t_i)K_{ab}/K_{ba}) & \text{if } 1 \le i \le N \\ (J(t_j) + [1 - I(t_j)]K_{ab}/K_{ba}) & \text{if } 1 \le j \le N \text{ with } j \equiv i - N \end{cases}. \tag{14.19}$$

In magnetization transfer problems it is often possible to take multiple independent measurements of the exchanging spins. For example one can invert the "a" site and then watch the effect of the relaxation on the "b" site spins. Similarly, one could invert the "b" site and then even invert both sites simultaneously. Consequently, we are going to adopt the notation, $d_j(t_i)$, to designate the ith data item of the jth inversion recovery. Similarly, M_{j1} will the initial "a" site magnetization for the jth inversion recovery. In what follows, it should be understood that different data sets may have different acquisitions times, even though we will not adopt a notation to represent this.

The joint posterior probability for the four parameters of interest is represented symbolically by $P(K_{ab}K_{ba}R_{1a}R_{1b}|DI)$, where D are the amplitudes or peak intensities for the "a" and "b" sites for *all* of the data sets. If we designate the posterior probability for the parameters computed from the jth data set as $P(K_{ab}K_{ba}R_{1a}R_{1b}|D_jI)$ then the posterior probability computed from all of the data is given by

$$P(K_{ab}K_{ba}R_{1a}R_{1b}|DI) = \prod_{j=1}^{m} P(K_{ab}K_{ba}R_{1a}R_{1b}|D_jI). \tag{14.20}$$

The right-hand side of this equation is computed from the joint posterior probability for all of the parameters:

$$P(K_{ab}K_{ba}R_{1a}R_{1b}|D_jI) = \int P(K_{ab}K_{ba}R_{1a}R_{1b}M_{j1}M_{j2}M_{j3}\sigma|D_jI)dM_{j1}dM_{j2}dM_{j3}d\sigma \tag{14.21}$$

where the amplitudes and standard deviation for the noise prior probability have been removed by marginalization. To compute the joint posterior probability for all of the parameters, we first factor the integrand using Bayes' theorem:

$$\begin{aligned} P(K_{ab}K_{ba}R_{1a}R_{1b}M_{j1}M_{j2}M_{j3}\sigma|D_jI) &\propto P(K_{ab}K_{ba}R_{1a}R_{1b}M_{j1}M_{j2}M_{j3}\sigma_j|I) \\ &\times P(D_j|K_{ab}K_{ba}R_{1a}R_{1b}M_{j1}M_{j2}M_{j3}\sigma_jI). \end{aligned} \tag{14.22}$$

Next the joint prior probability for the parameters, $P(K_{ab}K_{ba}R_{1a}R_{1b}M_{j1}M_{j2}M_{j3}\sigma_j|I)$, is factored into a series of independent priors for each of the parameters:

$$\begin{aligned} P(K_{ab}K_{ba}R_{1a}R_{1b}M_{j1}M_{j2}M_{j3}\sigma_j|I) &= P(K_{ab}|I)P(K_{ba}|I)P(R_{1a}|I)P(R_{1b}|I) \\ &\times P(M_{j1}|I)P(M_{j2}|I)P(M_{j3}|I)P(\sigma_j|I). \end{aligned} \tag{14.23}$$

Using Eqs. (14.23,14.22,14.21 and 14.20), one obtains,

$$\begin{aligned} P(K_{ab}K_{ba}R_{1a}R_{1b}|DI) &= P(K_{ab}|I)P(K_{ba}|I)P(R_{1a}|I)P(R_{1b}|I) \\ &\times \prod_{j=1}^{m}\Bigg[\int dM_{j1}dM_{j2}dM_{j3}d\sigma_j P(\sigma_j|I) \\ &\quad \times P(M_{j1}|I)P(M_{j2}|I)P(M_{j3}|I) \\ &\quad \times P(D_j|K_{ab}K_{ba}R_{1a}R_{1b}M_{J1}M_{j2}M_{j3}\sigma_jI)\Bigg] \end{aligned} \tag{14.24}$$

as the posterior probability for the parameters of interest.

We have now reached the point in the calculation where we must assign numerical values to represent these probabilities. The prior probabilities for the four parameters of interest are assigned as Gaussians that are constructed out of the Low-High ranges that are input on the interface. If x denotes one of the four parameters of interest, then its prior probability is given by

$$P(x|I) \propto \begin{cases} \exp\left\{-\frac{(\text{Mean}-x)^2}{2\text{Sd}^2}\right\} & \text{if Low} \leq x \leq \text{High} \\ 0 & \text{otherwise} \end{cases} \tag{14.25}$$

where "Low" and "High" appropriate inputs from the interface, "Mean" is the average of the low and high, and "Sd" is set so that the High-Low interval represents a 3 standard deviation interval.

The prior probabilities for the standard deviation of the noise was assigned as a Jeffreys' prior, $1/\sigma_j$. The prior probability for the amplitudes was assigned using a uniform prior probability. Finally, the likelihoods were assigned using a Gaussian of standard deviation σ_j, one obtains

$$\begin{aligned} P(K_{ab}K_{ba}R_{1a}R_{1b}|DI) &\propto P(K_{ab}|I)P(K_{ba}|I)P(R_{1a}|I)P(R_{1b}|I) \\ &\times \prod_{j=1}^{m}\left[\int dM_{j1}dM_{j2}dM_{j3}\frac{d\sigma_j}{\sigma_j}\left(2\pi\sigma_j^2\right)^{-N}\exp\left\{-\frac{Q_j}{2\sigma_j^2}\right\}\right] \end{aligned} \tag{14.26}$$

where we have left the four prior probabilities for the parameters of interest in their symbolic form, and

$$\begin{aligned} Q_j &\equiv \sum_{i=1}^{2N}\left[d_j(t_i) - \sum_{\ell=1}^{3}M_{j\ell}\mathcal{H}_j(t_i)\right]^2 \\ &= 2N_j(\overline{d^2})_j - 2\sum_{\ell=1}^{3}M_{j\ell}T_{j\ell} + \sum_{k=1}^{3}\sum_{l=1}^{3}(g_{kl})_j M_{jk}M_{jl}. \end{aligned} \tag{14.27}$$

The mean-squared data value, $(\overline{d^2})_j$, for the jth inversion is defined as

$$(\overline{d^2})_j = \frac{1}{2N_j}\sum_{i=1}^{2N_j} d_j(t_i)^2 \equiv \frac{1}{2N_j}\sum_{i=1}^{N_j} d_{aj}(t_i)^2 + d_{bj}(t_i)^2 \tag{14.28}$$

where N_j is the number of complex data values in the jth inversion. The projection of the ℓth model function onto the jth inversion, $T_{j\ell}$, is given by

$$T_{j\ell} = \sum_{i=1}^{2N_j} d_j(t_i)\mathcal{H}_{j\ell}(t_i). \tag{14.29}$$

The matrix $(g_{kl})_j$ is defined by

$$(g_{kl})_j \equiv \sum_{i=1}^{2N_j}\mathcal{H}_{jk}(t_i)\mathcal{H}_{j\ell}(t_i). \tag{14.30}$$

This matrix will depend on the individual inversion if the delay times differ from one inversion to another.

Evaluating the integrals over the amplitudes and standard deviations is straightforward, if not tedious. Evaluating the amplitude integrals one obtains:

$$\begin{aligned} P(K_{ab}K_{ba}R_{1a}R_{1b}|DI) &\propto P(K_{ab}|I)P(K_{ba}|I)P(R_{1a}|I)P(R_{1b}|I) \\ &\times \prod_{j=1}^{m}\int\frac{d\sigma_j}{\sigma_j}\left|g_{kl}\right|_j^{-\frac{1}{2}}\left(2\pi\sigma_j^2\right)^{-N+3}\exp\left\{-\frac{2N_j(\overline{d^2})_j - (\overline{h^2})_j}{2\sigma_j^2}\right\} \end{aligned} \tag{14.31}$$

where $|g_{kl}|_j$ is the determinant of the $(g_{jk})_j$ matrix. The sufficient statistic, $(\overline{h^2})_j$, is the total-squared projection of the model onto the data for the jth inversion:

$$(\overline{h^2})_j = \sum_{k=1}^{3} T_{kj} \hat{M}_{kj}. \tag{14.32}$$

The $\hat{M}_{kj}$, are given by the solution to the following linear set of equations:

$$\sum_{k=1}^{3} (g_{lk})_j \hat{M}_{kj} = T_{lj} \qquad (1 \le l \le 3). \tag{14.33}$$

The integrals over the standard deviations of the noise prior probabilities may all be transformed into Gamma functions and evaluating such integrals is straightforward, one obtains

$$\begin{aligned} P(K_{ab}K_{ba}R_{1a}R_{1b}|D_aD_bI) \quad &\propto \quad P(K_{ab}|I)P(K_{ba}|I)P(R_{1a}|I)P(R_{1b}|I) \\ &\times \quad \prod_{j=1}^{m} |g_{kl}|_j^{-\frac{1}{2}} \left[2N_j(\overline{d^2})_j - (\overline{h^2})_j\right]^{\frac{3-N_j}{2}} \end{aligned} \tag{14.34}$$

where we have dropped a number of constants that cancel when this distribution is normalized.

Markov chain Monte Carlo with simulated annealing is used to draw samples from the joint posterior probability for K_{ab}, K_{ba}, R_{1a} and R_{1b}, Eq. (14.34). These samples are used to approximate the marginal posterior probability for each of the parameters separately. In addition, the program also uses these samples to form an approximation to the posterior probability for the volume fractions,

$$p_a = \frac{K_{ba}}{K_{ab} + K_{ba}} \quad \text{and} \quad p_b = \frac{K_{ab}}{K_{ab} + K_{ba}}, \tag{14.35}$$

the exchange times,

$$\tau_{ab} = \frac{1}{K_{ab}} \quad \text{and} \quad \tau_{ba} = \frac{1}{K_{ba}}, \tag{14.36}$$

and the relaxation times,

$$T_{1a} = \frac{1}{R_{1a}} \quad \text{and} \quad T_{1b} = \frac{1}{R_{1b}}. \tag{14.37}$$

Note that in each of these calculations involves a change of variables of the form $Y = 1/X$. This change of variables introduces a factor of the form $dY = -dXX^{-2}$ into the posterior. This factor shift the location of the maximum posterior probability between the paired variables. Consequently, the maximum posterior probability estimate for Y is not in general equal to $1/X$.

14.2 Using The Package

The Text outputs files from the Magnetization Transfer packages consist of: “Bayes.prob.model,” “MtZ.mcmc.values,” “Bayes.params,” “Console.log,” “Bayes.accepted” and a “Bayes.Condensed.File.” These output files can be viewed using the Text Viewer or they can be viewed using File Viewer by navigating to the current working directory and then selecting the files. The format of the

Figure 14.2: Magnetization Transfer Package Peak Picking

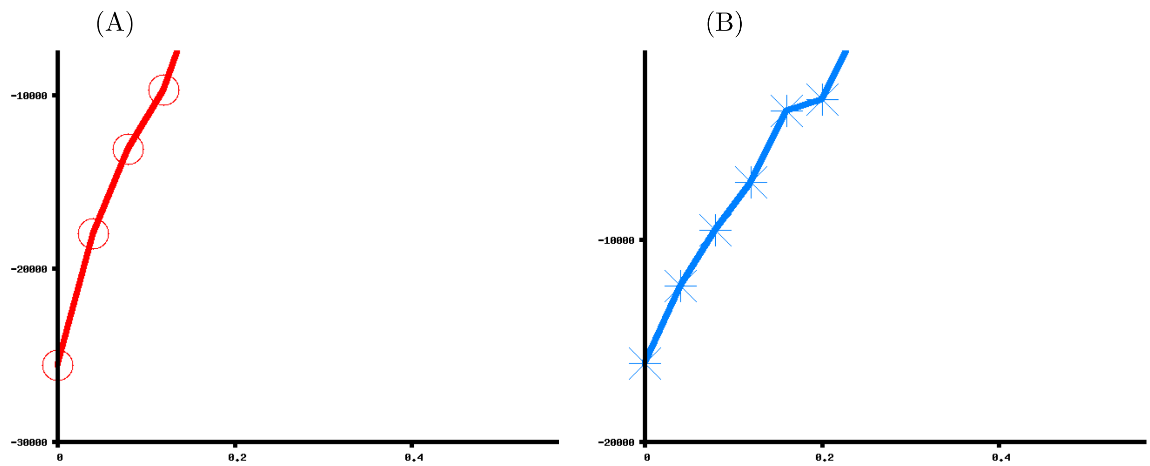

Figure 14.2: The peak intensities of the exchanging sites are analyzed by the magnetization exchange package, consequently, as illustrated here, the data are three column Ascii: a time, and two peak intensities. These peak intensities may be loaded from a peak pick, a Bayes Analyze run, or from an Ascii file. The example shown in this figure is from an peak pick. Panel (A) is the peak intensities when the left-hand peak was inverted and Panel (B) is the peak intensities when the right-hand peak was inverted. The data shown in Panel (A) was generated using a peak pick of the inversion recover spectrum shown in Figure 14.3.

mcmc.values report is discussed in Appendix D and the other reports are discussed in Chapter 3. Additionally, the "Plot Results Viewer" can be used to view the output probability density functions. In addition to the standard data, model and residual plots there are probability density functions for the decay rate constants, decay times, the amplitudes for each data set for each exponential and finally there are probability density functions for the standard deviation of the noise in each data set.

The data used by this package can be multiple three column Ascii files, see Fig. 14.2 for an example of this data. The data consists of a time axis and the left and right-hand peak intensity from an inversion recover experiment. The data can be loaded in one of three ways: First, a three column Ascii file can be directly loaded using the Files menu; Second, The spectrum of a magnetization transfer inversion recovery Fid can be loaded and the peak amplitudes can be extracted and loaded. Third, the "File/Load Ascii/Bayes Analyze File" button can be used to extract the peak amplitudes from the currently loaded Bayes Analyze files. If Bayes Analyze has not been run on this Fid, you must run it before you can use this option.

Figure 14.3 is the first trace in the spectrum of the inversion recover used to generate the data shown in Fig. 14.2(A). Figure 14.4 is a plot of the spectrum of the two exchanging resonances for each delay time in the inversion recover experiment shown in Fig. 14.3. Note how the left-hand resonances starts inverted and as a function of the delay time it rather quickly recovers. If you examine Fig. 14.4, which is a VnmrJ dssh display of the region around the two exchanging peaks, you can easily see that, initially both peaks have reduced amplitude and as the left-hand peak recovers, both peaks

Figure 14.3: Magnetization Transfer Example Data

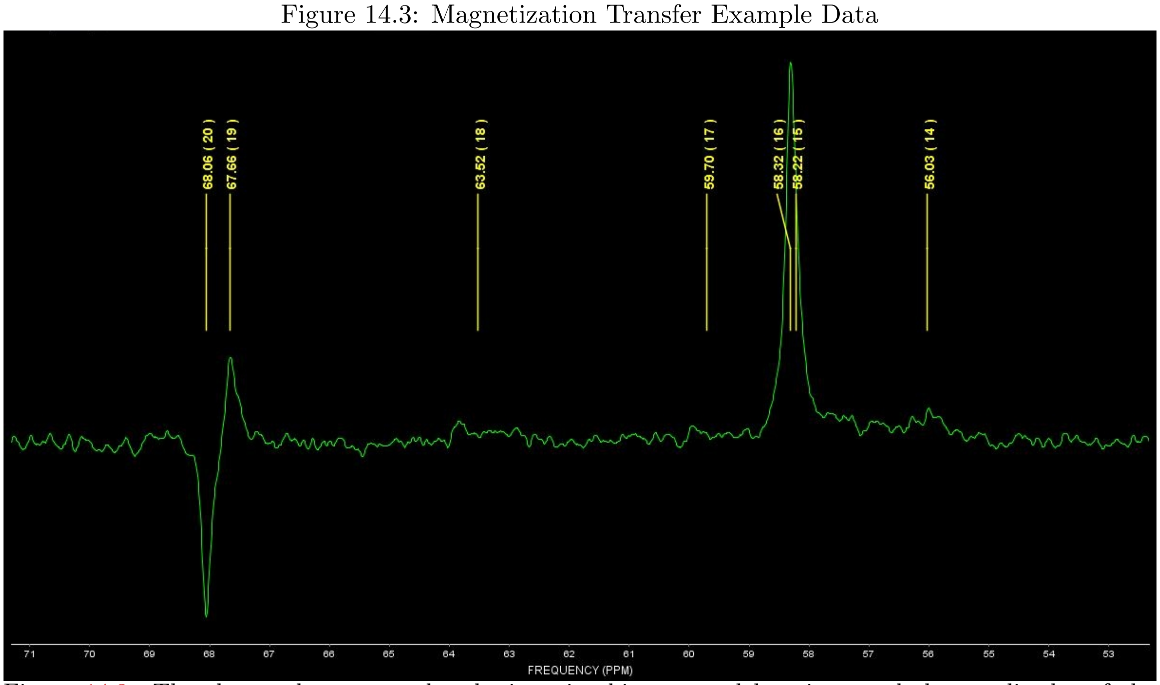

Figure 14.3: The three columns are the abscissa, in this case a delay time, and the amplitudes of the resonances of the A and B Sites. In this spectrum Site A is the resonance near 68PPM, and Site B is near 67.66PPM. To load this data, place a double cursor on each resonance and hit the "Get Peak" button in the lower right. Alternately, If Bayes Analyze has been run on this data, the "File/Load Ascii/Bayes Analyze File" menu can be used to load the resonance amplitudes from the Bayes Analyze files.

Figure 14.4: Magnetization Transfer Example Spectrum

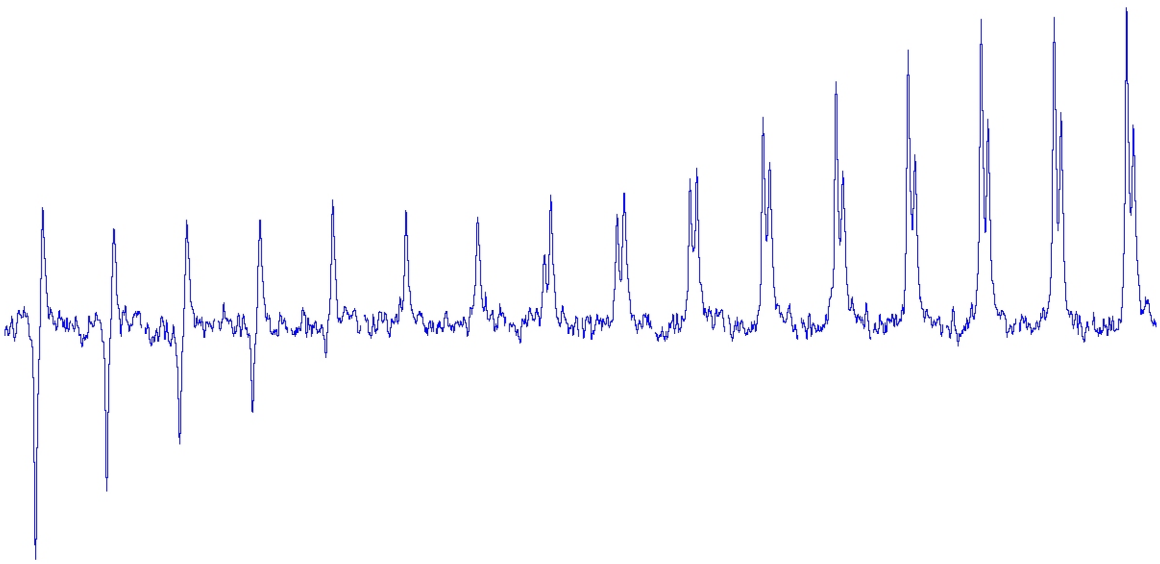

Figure 14.4: These spectra are a typical example of magnetization transfer data. Here the left-hand peak was selectively inverted and allow to recover. The data analyzed by the magnetization transfer package is the peak intensity or amplitude of the two sites exchanging magnetization. These peak intensity may be loaded using the File menu, extracted using a double cursor and the Get Peak button, or Bayes Analyze can be used to estimate the amplitudes, and these amplitudes can be loaded using the File/Ascii File/Bayes Analyze menu.

increase in intensity. In the three column Ascii data shown in Fig 14.2(A) the left-hand peak shown in Fig 14.3 was selectively inverted and then allowed to relax back to equilibrium. It is the peak intensities of the two resonances exchanging magnetization that are analyzed by the magnetization package.

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