MagProp User Manual

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Program Function

Visualisation and modelling of magnetic data

Program Features

Reading in Magnetic Data

Magnetic Data may either be imported directly from a SQUID File using the "Import SQUID File" module (described separately), or from an ascii file consisting of 2 or 3 column data. If the file comprises 2 column data the program will assume that one column corresponds to '*temperature*' and the other to '*ChiT*', '*Chi*' or '*ueff*'. If the file comprises 3 column data, the program will assume that the three columns correspond to '*temperature*', '*magnetisation*' and '*field*'. The user has to specify which column corresponds to which quantity. The quantity that is displayed and modelled can be changed at run time (see 'Program Options').

Entering a Model Hamiltonian

There are three ways in which to enter a model Hamiltonian. One way is to use the '*Hamiltonian Matrix Generator*', the help manual for which is provided separately. The second is to import ligand-field matrices in the form of a LIGFIELD text file. The LIGFIELD program may be obtained directly from the author Jesper Bendix. The third way is to import matrices as text files. This requires a little explanation: Lines within the text files beginning with # are understood to be comments. Only the top right hand corner of the matrix is entered. The matrix elements are listed by, *Row Index, Column Index, Matrix Element*. Following the formalism of the celebrated Faroese chemist Høgni Weihe, the matrix elements may be given in one of two ways. Consider the two different ways of entering the matrix element $\langle 1|1+2i|2\rangle$:

Format 1

```
1       2       1+2i

# Format 2
1       2       1       real
1       2       2       imaginary
```

As an example, consider the matrix,

$$\begin{pmatrix} \frac{D}{3}+g_z\beta B_z & \frac{g_x\beta B_x}{\sqrt{2}}-\frac{ig_y\beta B_y}{\sqrt{2}} & E \\ \frac{g_x\beta B_x}{\sqrt{2}}+\frac{ig_y\beta B_y}{\sqrt{2}} & -\frac{2D}{3} & \frac{g_x\beta B_x}{\sqrt{2}}-\frac{ig_y\beta B_y}{\sqrt{2}} \\ E & \frac{g_x\beta B_x}{\sqrt{2}}+\frac{ig_y\beta B_y}{\sqrt{2}} & \frac{D}{3}-g_z\beta B_z \end{pmatrix} \quad (1)$$

Following format 1, the content of the five files required to store matrix (1) are:

```
#       Filename D.mat
1       1       0.33333333333
2       2      -0.66666666666
3       3       0.33333333333

#       Filename E.mat
1       3       1.0

#       Filename gz.mat
1       1       1.0
3       3      -1.0

#       Filename gx.mat
1       2       0.7071067812
2       3       0.7071067812

#       Filename gy.mat
1       2       -0.7071067812i
2       3       -0.7071067812i
```

When entering these matrix files, the user must specify which are to be multiplied by B_z, B_x and B_y. Note that Bohr Magneton is incorporated into the field *B*. As well as specifying the filename, the user is prompted to enter a designation for the term in the matrix. The zero-field terms are entered separately.

Worked Example of how to Model Magnetic Data

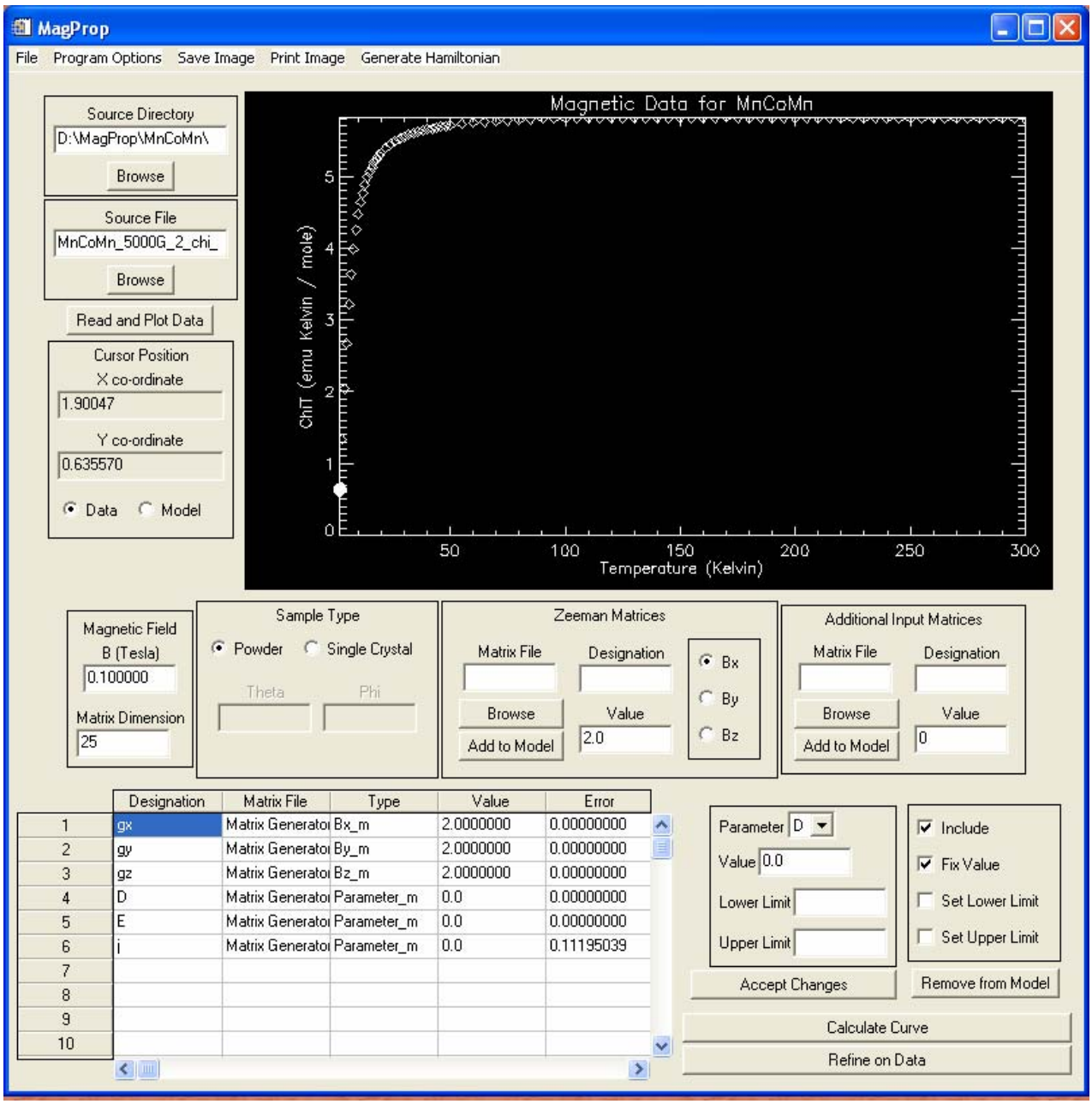
We consider the magnetic properties of a Mn-Co-Mn linear trimer, in which all the transition metal ions are in the +3 oxidation state. The model Hamiltonian may be written as,

$$\hat{H} = D\sum\nolimits_{1,2}\left(\hat{S}_{iz}^2 - \tfrac{1}{3}S_i\left(S_i+1\right)\right) + E\sum_{1,2}\left(\hat{S}_{ix}^2 - \hat{S}_{iy}^2\right) + \sum_{1,2} B\cdot g\cdot\hat{S}_i + J\hat{S}_1\cdot\hat{S}_2\,,$$

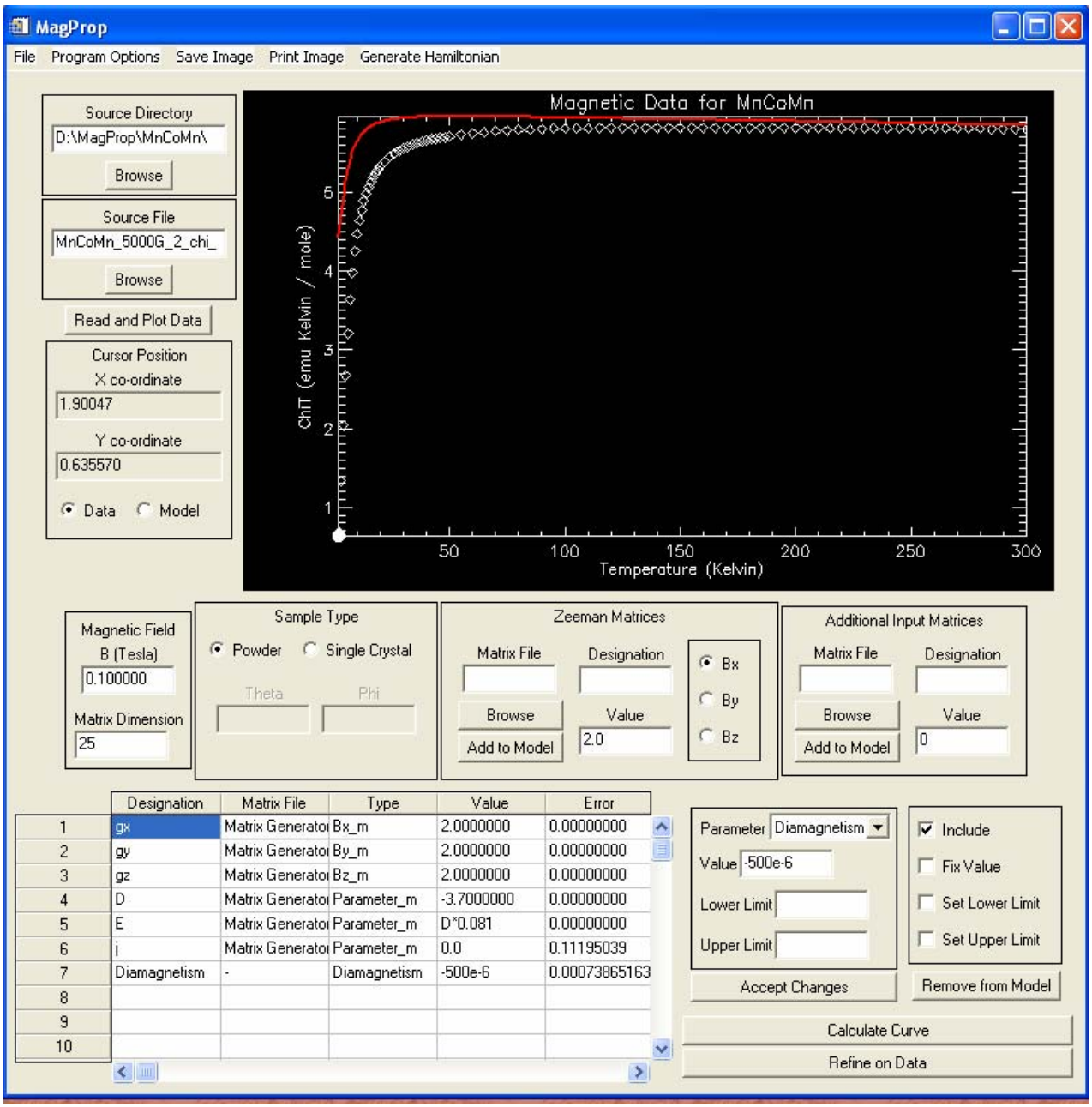
where the indices 1 and 2 run over the manganese(III) cations.

The manganese(III) are crystallographically equivalent and inelastic neutron scattering measurements suggest that the single ion anisotropy of the manganese(III) centres is well described by the parameters D=-3.7 cm^{-1}, E = 0.3 cm^{-1}. Variable temperature susceptibility data have been collected but the diamagnetic susceptibility cannot be estimated with an adequate degree of certainty, owing to the complexity of the compound.

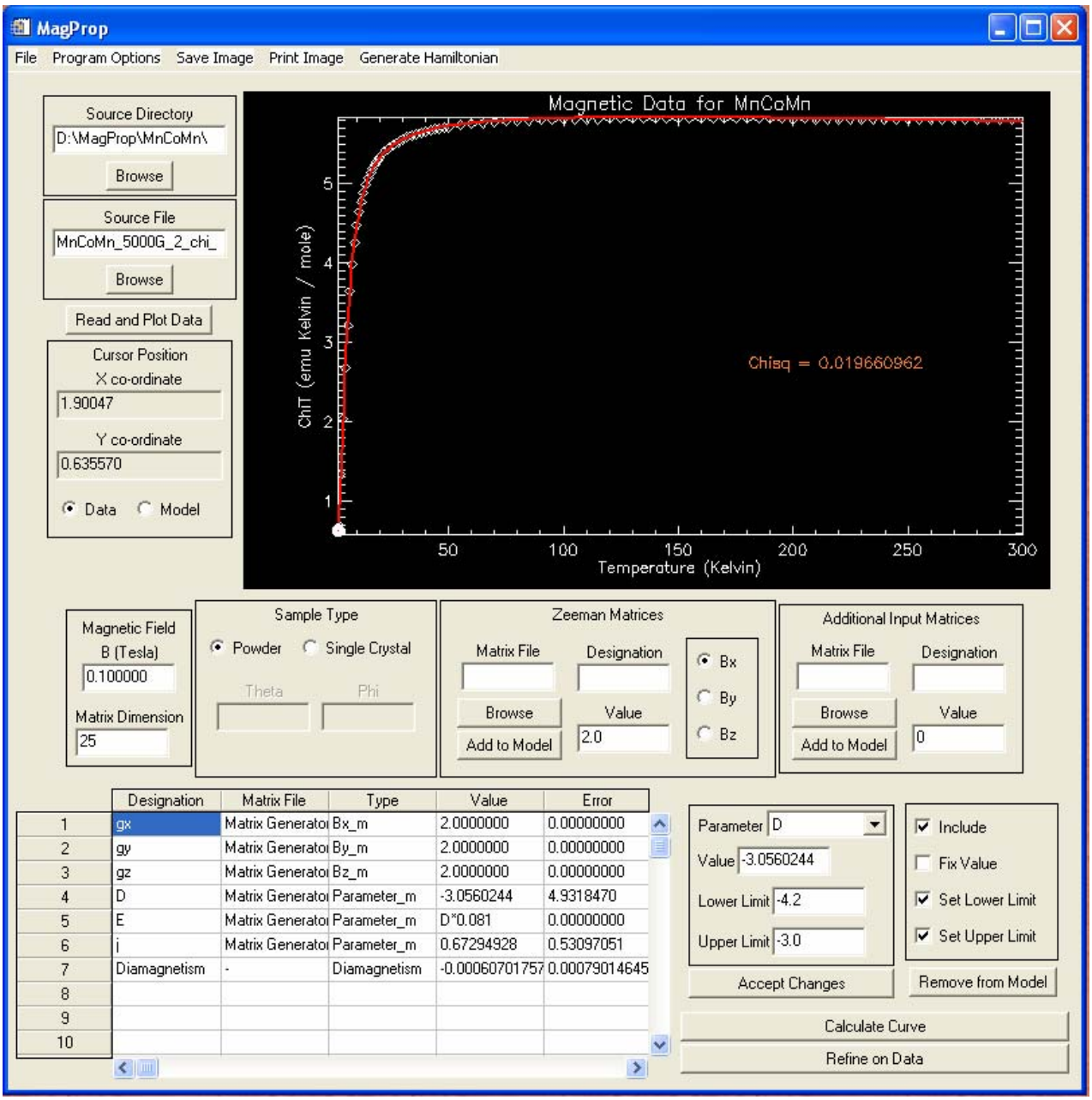
We join the session after the SQUID data have been worked up using the *Import SQUID File* utility – no diamagnetic correction having been applied – and the matrices constructed and imported using the *Hamiltonian Matrix Generator* program.



Let us suppose we wish to hold the *E/D* ratio constant at 0.3/-3.7 = -0.081. A value of -3.7 cm^{-1} is entered for *D* and *E* is fixed at *D**0.081. The g values are fixed at 2.0 and a diamagnetic correction is included in the model, with an initial estimate of $-500*10^{-6}$ emu /mole. Upon pressing the *Calculate Curve* button, the GUI looks like this:



We now wish to refine on the data with this model, confining the parameter *D* between the limits of -3.0 and -4.2 cm^{-1}. As shown below, the fit is excellent but the parameters poorly defined. The user may introduce intermolecular exchange interactions, refine on the data within a given temperature range, define the diagonalisation algorithm, add error bars, define how the powder average is calculated and define how the data are refined. See *Program Options* for further details. I like to think that you can learn how to use the program simply by playing around so please give it a go.


MagProp
File
Program Options
Save Image
Print Image
Generate Hamiltonian
Source Directory
D:\MagProp\MnCoMn\
Browse
Source File
MnCoMn_5000G_2_chi_
Browse
Read and Plot Data
Cursor Position
X co-ordinate
1.90047
Y co-ordinate
0.635570
Data
Model
Magnetic Data for MnCoMn
ChiT (emu Kelvin / mole)
Temperature (Kelvin)
Chisq = 0.019660962
Magnetic Field
B (Tesla)
0.100000
Matrix Dimension
25
Sample Type
Powder
Single Crystal
Theta
Phi
Zeeman Matrices
Matrix File
Designation
Browse
Add to Model
Value
2.0
Bx
By
Bz
Additional Input Matrices
Matrix File
Designation
Browse
Add to Model
Value
0
Designation
Matrix File
Type
Value
Error
1 gx Matrix Generator Bx_m 2.0000000 0.00000000
2 gy Matrix Generator By_m 2.0000000 0.00000000
3 gz Matrix Generator Bz_m 2.0000000 0.00000000
4 D Matrix Generator Parameter_m -3.0560244 4.9318470
5 E Matrix Generator Parameter_m D*0.081 0.00000000
6 i Matrix Generator Parameter_m 0.67294928 0.53097051
7 Diamagnetism - Diamagnetism -0.00060701757 0.00079014645
8
9
10
Parameter D
Value -3.0560244
Lower Limit -4.2
Upper Limit -3.0
Include
Fix Value
Set Lower Limit
Set Upper Limit
Accept Changes
Remove from Model
Calculate Curve
Refine on Data