DTA2dat GUI

1. Introduction

DTA2dat GUI is a Graphical User Interface (GUI) for MATLAB to convert .DTA-files generated by Bruker EPR Spectrometers into ASCII-files (.dat). Currently, it can cope with 1D and 2D .DTA-files (e.g. 1D Field Sweep and 2D Power Plot).

Key features:

- Conversion of 1D and 2D .DTA-files into ASCII-files (.dat). It is possible to select either one single file or to convert all files in a folder.
- Transformation of the magnetic field axis into g-scale and shift of the microwave frequency, e.g. to compensate for frequency drifts among different individual spectra before overlay.
- Mirror symmetric PDS traces (e.g. DQC and SIFTER) at the point of maximum signal.

These functions are described in detail below.

2. Requirements

The minimum requirements to run the script are:

- Installation of MATLAB ≥ version R2018a.
- Proper path setting of the EasySpin package[1] within MATLAB.

3. Description of the program

As all MATLAB scripts, the program can be started by either clicking the "Run" button in the task bar of MATLAB or by pressing the "F5" key. This opens a Graphical User Interface (GUI). The options available herein are described below.

Select File: Press this button to process a single .DTA-file. If none of the options listed below is selected, a simple conversion of a 1D .DTA-file to .dat will be performed.

Select Folder: Press this button to process all .DTA-files within a folder. If none of the options listed below is selected, a simple conversion of all 1D .DTA-files to .dat will be performed.

Options for conversion of 2-dimensional .DTA-files:

- Save separate .dat-files: Each slice of the .DTA-file will be saved as a separate .dat-file.
- Save concatenated .dat-file: All slices of the .DTA-file will be saved in a single .dat-file. Herein, the first column contains the x-values and the following columns contain the y-values of the different slices. In addition to the spectral data (e.g. magnetic field and intensity), the third quantity (e.g. microwave power, temperature etc.) will be exported as a _params.dat-file. It contains the respective value of this third quantity for each slice.
- If none of the options related to 2D .DTA-files is selected, 2D .DTA-files will not be processed.

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[1] S. Stoll, A. Schweiger, *J. Magn. Reson.* **2006**, *178*, 42–55. EasySpin can be downloaded at www.easyspin.org

Options for frequency shifting and g-scale conversion

- **Save raw data as .dat-file:** Simple conversion of .DTA to .dat-file.
- **Save as g-scale:** The magnetic field axis will be converted to g-scale using the frequency given in the .DSC-file.
- **Save at target frequency (in GHz):** Shifts the magnetic field axis. This option can be used to overlay spectra recorded at slightly different frequencies.
- Note that g-scale transformation and frequency shifting is currently available only for 1D field swept EPR spectra!

Options for mirroring PDS-traces

- **Save raw data as .dat-file:** Simple conversion of .DTA to .dat-file.
- **Mirror PDS-trace at maximum:** Mirrors symmetric PDS-traces (e.g. DQC) at the time when the maximum signal amplitude occurs.