MossWinn Internet Database

Manual

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1. Introduction

The MossWinn Internet Database (MIDB) is a Mossbauer spectroscopy database system service that can be accessed via the internet by the help of the MossWinn program. Full access to the database requires subscription to the MossWinn Services (see http://www.mosswinn.hu/mws.htm), whereas **free query and browse access** to the database is provided via the **DTB** menubox in the main menu of MossWinn. The MIDB is intended to serve as

- a tool for information exchange among Mossbauer spectroscopists,
- a starting point for Mossbauer literature surveys,
- a starting point for Mossbauer data surveys, and as
- a model library, i.e. a starting point for database aided Mossbauer spectrum analysis.

The MossWinn Internet Database enables subscribers to

- **publish** their own database records in the MIDB,
- **query & browse** the records included in the MIDB,
- **withdraw** or **edit** their own database records published in the MIDB,
- **find database match(es)** for their own spectrum under analysis, and
- **reuse fit models included in database records** to fit own spectra.

The functions of the database system can be accessed via the submenu items of the **DB** menu box in the **FIT** menu (see page 4), whereas some of the functions are also available directly from the main menu via the **DTB** and **EDT** menu boxes. The manual of MossWinn can be consulted concerning the access of the latter functions.

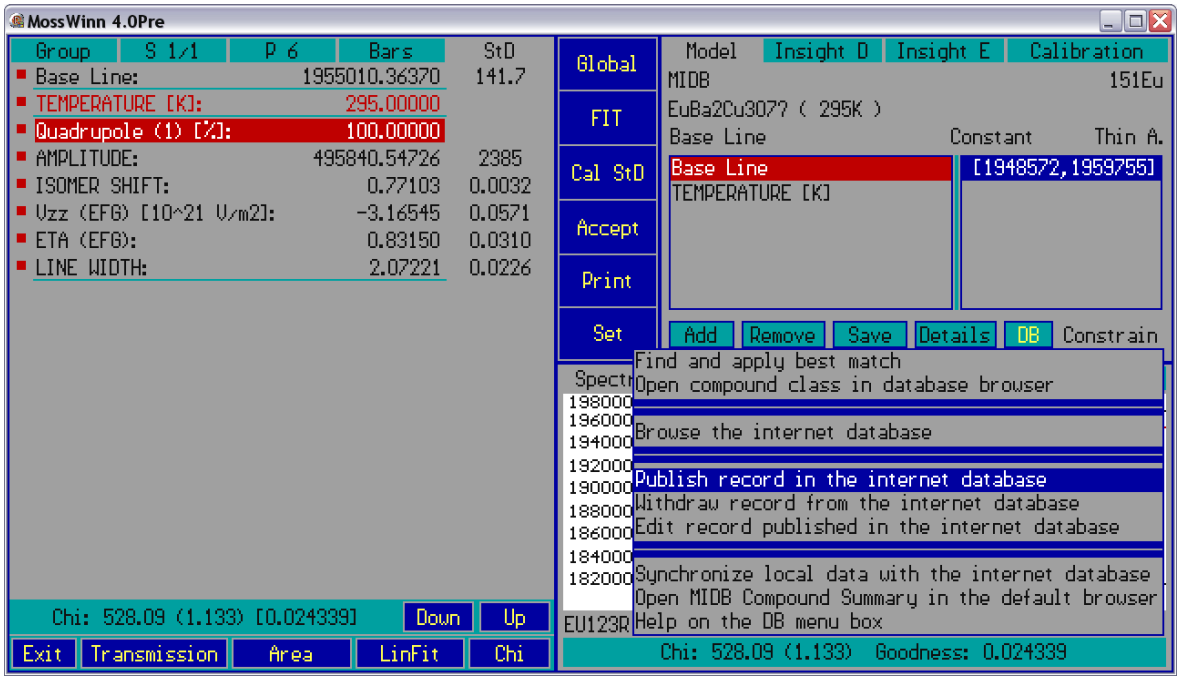
MossWinn's internet connections

Internet related functions offered by MossWinn are performed by the establishment of connections to several different internet resources/servers. Users who have a **firewall** installed on their PC system may experience warnings related to these connections when MossWinn starts. In order to avoid such warnings, one needs to include MossWinn's connections into the 'whitelist' of the firewall software. In case of doubt, please, do not hesitate to contact the author for detailed information.

Functions of MossWinn that require the establishment of internet connections can be enabled/disabled via the **Set internet access options** submenu of the **SET** menu box in the main menu.

2. Accessing the functions of the MIDB database

In order to access the functions of the database, load a spectrum and enter the **FIT** menu. The **DB** menu box of the **FIT** menu provides access to the functions of the MossWinn Internet Database as follows.



Find and apply best match - Turn to this option in order to search through the database records in order to find the spectrum that best matches the fitted spectrum currently on the screen, and to set the corresponding fit model as included in the database record returned by the search. (The currently set fit model will be overwritten.) The fitness of the database records with respect to the current spectrum is evaluated by considering the isomer shift of the default isomer shift reference material (associated with the current source nuclide) that can be set via the **Default isomer shift reference** submenu option of the **SET** menu. The search can be performed via the following submenu options (a press directly on the **Find and apply best match** menu item is equivalent to the option **Considering own records**):

- **Considering own records** - The search will consider only those records that were published in the database by using the hardware key that is currently attached to the computer.
- **Considering all records** - The search will consider all database records.
- **Considering all transmission (reflection) type records** - The search will consider only those database records that refer to measurements carried out in transmission (reflection) geometry.

The fit model returned as the best match will be saved automatically as a new model of the **MIDB [*]** model group where * stands for the corresponding source nuclide. Apart from the best match, the search will also return several further records in descending order of their fitness.

Select this menu again in order to see the corresponding list and apply another one of the returned records.

Open compound class in database browser - Turn to this option in order to select one of the records returned by the **Find and apply best match** function, and open the corresponding compound class in the database browser.

Browse the internet database - Select this option in order to display the database browser (see page 18) that allows one to search through the database records according to various criteria. The database browser also provides the possibility to try/apply the fit models, represented by the database records, to the fitted spectrum currently on the screen.

Publish record in the internet database - Select this option in order to publish the current fit model and/or a downsampled version of the current spectrum in the MossWinn Internet Database. If along with the fit parameters you also want to publish their standard deviation in the database, calculate the corresponding standard deviations via the **Cal StD** menu before turning to this option. Once the option is selected, first the Database record input form (see page 7) becomes displayed on which one can set various parameters associated with the record to be published. Then, the next form (see page 14) provides the possibility to set the resampled form of the measured spectrum, and to declare whether one wants to publish only the fit model, only the resampled spectrum, or both. On the next form (see page 16) a preview of the record is displayed, where one can check how the record will appear when published. The record becomes finally published when on the preview form the **Publish record** button is pressed. Once a record is published in the database, it may appear in the MIDB database browser of MIDB subscribers all around the world. The **MIDB Publisher's Guide** (`http://www.mosswinn.hu/midbguide.htm`) contains further information concerning the publication of MIDB records.

Withdraw record from the internet database - Select this option in order to withdraw a MIDB record published earlier by using the hardware key that is currently attached to the computer (*own record*). The own record that is to be withdrawn can be selected on the appearing **MIDB browser** form (see page 29). *Withdrawal of own records from the MIDB database does not require subscription to the database.*

Edit record published in the internet database - Select this option to edit one of the own MIDB records by changing the record parameters that can be set on the **Database record input form**. The fit model and the resampled spectrum associated with the record cannot be edited in this way. The own record that is to be edited can be selected on the appearing **MIDB browser** form (see page 29).

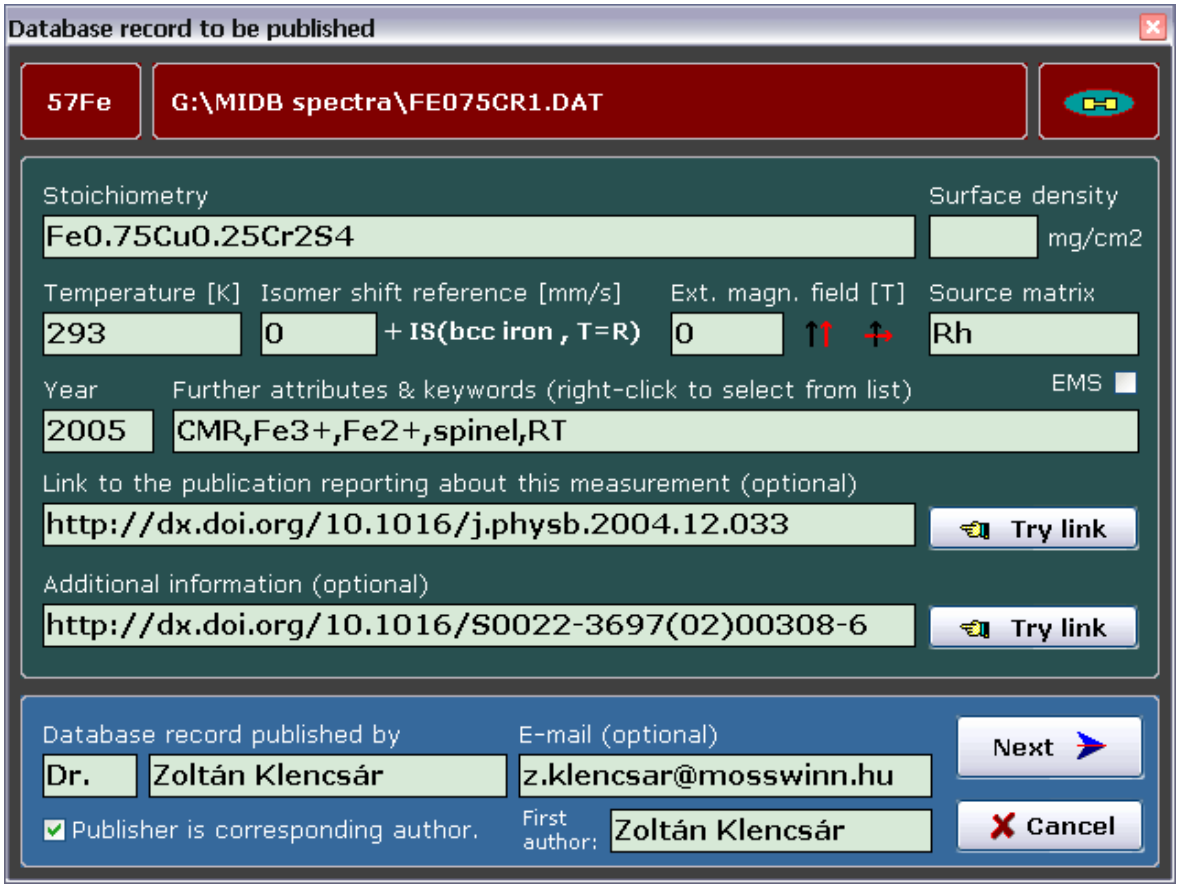
Synchronize local data with the internet database - Select this option to carry out pending MIDB publication and withdrawal operations, and to synchronize local data with the MIDB host server. The frequency of such synchronization events may be subject to a limitation.

Open MIDB Compound Summary in the default browser - Select this option to open the MIDB Compound Summary in the default browser (`http://www.mosswinn.hu/midbsummary.htm`).

Help on the DB menu box - Select this option to bring up the html help concerning the **DB** menu box.

3. The database record input form

Each record published in the database is associated with a certain Mossbauer spectrum and the corresponding fit model as set by the user in the **FIT** menu of MossWinn.



Concerning the Mossbauer spectrum, the record can include the following user-provided information:

- Stoichiometry of the measured compound (**required**).
- Total surface density of the measured sample (optional).
- Temperature of the measurement (**required**).
- Flux density of the external magnetic field applied to the sample during the measurement (**required**). (Assumed to be zero if the field is empty.)
- Magnetic field orientation with respect to the gamma ray (optional).
- Isomer shift of the IS reference material (whose isomer shift would be 0 mm/s on the spectrum's velocity scale) given relative to the standard IS reference material (**required**).
- Source matrix (or absorber material in case of EMS measurements) applied in the measurement (optional).
- Publication year of the associated paper or the year of measurement in the absence of publication (optional).

- Internet link to the associated publication's official site (optional).
- Additional textual information or internet link to a website containing additional information concerning the measurement (optional).
- Keywords and further attributes associated with the measurement (optional).
- Name of the publisher (**required**).
- Title of the publisher (optional).
- E-mail of the publisher (optional).
- Name of the first author of the associated publication (**required**).

At least one of the following items is required to be present in the database record:*

- Fit model associated with the measured spectrum (optional*).
- Downsampled version of the measured spectrum (optional*).

In order to publish a database record for a spectrum, select the spectrum to be red-framed in the main menu, and enter the Fit menu. Fit the spectrum and calculate the standard deviation of the fitted parameter values via the **Cal StD** menu box. (If the latter step is skipped, the StD values will not be included in the published record.) Then, select the **Publish record in the internet database** submenu of the **DB** menu (see page 4). As a result, the **Database record input form** appears.

- **Source nuclide** - Shows the source nuclide that was set in the **FIT** menu for the current spectrum.
- **Spectrum file** - Shows the path and name of the data file that contains the spectrum associated with the record to be published. (Information on the path and name of the file will not be included in the published record.)
- **Help** - Press on the help ellipse in order to open this help in the default browser.
- **Stoichiometry of the sample** - The stoichiometry of the sample associated with the record should be entered in this edit box (*required field*). (If the *stoichiometry* special parameter was set for the current spectrum, then MossWinn will automatically fill out this edit box with the corresponding information.) ***Element symbols*** and quantities should be written in accordance with the usual writing style, e.g. **Fe3O4**. In ambiguous cases the case of the symbol letters is relevant. For example **Co** and **CO** are interpreted as cobalt and carbon monoxide, respectively. Similarly, **Cas** = **CaS** = **Ca** + **S**, **CAS** = **CAs** = **C** + **As**, **SRY** = **SrY** = **Sr** + **Y**. The rule is that if disregarding the case a double-char can be interpreted as one element symbol, then it is interpreted that way when **(1)** the first character cannot correspond to an element symbol alone, or **(2)** the second character is written with lower case, or **(3)** the second character cannot be interpreted as an element symbol - neither alone nor together with the next character. (The stoichiometry is evaluated from

left to right.) It is recommended to use the correct case in order to avoid ambiguity. ***Quantities*** can be written after the element symbols or after subunits designated by ***parentheses***/square brackets — **( )** and **[ ]** types can be used equivalently, also in a nested way —, or before molecular units as in **6H2O**. In the latter case the scope of multiplication includes the largest possible molecular unit directly following the multiplicator. Quantities can also be given as ***fractions*** as in the case **La1/3Sr2/3FeO3** (displayed as $La_{1/3}Sr_{2/3}FeO_3$). The multiplication sign ***** can be used to denote, e.g., hydrous compounds such as in **Fe2O3*1/2H2O** that would be displayed as $Fe_2O_3 \cdot 1/2H_2O$. Any text can be inserted in the stoichiometry by using double quotes, e.g. **"Cis-"Fe(NH3)2F4** that would be displayed in the database browser as Cis-$Fe(NH_3)_2F_4$. Text between double quotes can be formatted by using HTML-style formatting elements such as **** for *italic*, **** for **bold**, **<u></u>** for underline, **** for subscript and **** for superscript text style. HTML code can also be used between double quotes to display ***greek letters*** (e.g. **α β** for α β) in stoichiometry formulas such as **"γ-"Fe2O3** (displayed as γ-Fe_2O_3). ***Mass numbers*** are interpreted only for the following nuclides (*allowed isotopes*): **^{57}Fe**, **^{57}Co**, **^{119}Sn**, **^{151}Eu**, **^{125}Te**, **^{121}Sb**, **^{129}I**, **^{141}Pr**, **^{237}Np**, **^{161}Dy**, **^{197}Au**. For allowed isotopes a number is interpreted as mass number if it is preceeded by a space and it is directly followed by the corresponding element symbol. ***Mixtures*** may be denoted by using the **+** sign. For example, **(Fe3O4)0.8 + ("α-"FeOOH)0.2** will be displayed as $(Fe_3O_4)_{0.8}$ + $(\alpha\text{-FeOOH})_{0.2}$, i.e. 80% magnetite and 20% goethite (molar percent). It is recommended to write the formula of mixtures by the indication of the molar fractions of the individual compounds, as in the example above. ***Uncertain quantities*** may be denoted by a question mark **?** written after the uncertain quantity, e.g. as in **EuBa2Cu3O7?** (being displayed as $EuBa_2Cu_3O_{7?}$ in the database browser), with the meaning being equivalent to $EuBa_2Cu_3O_{7-\delta}$. If there are ***unknown quantities*** in the stoichiometry, write them as usual, without regard to whether the stoichiometric quantities are interpreted correctly by MossWinn or not. For example, a magnetite structure with altogether 10% Co and Ni could be written as **[Fe0.9(Co,Ni)0.1]3O4** if the atomic ratio of Co and Ni is unknown. This would be displayed as $[Fe_{0.9}(Co,Ni)_{0.1}]_3O_4$, and would be interpreted (unlike its usual meaning) as $[Fe_{0.9}Co_{0.1}Ni_{0.1}]_3O_4$ internally. Instead of an accurate chemical formula a **symbolic name** may also be given between double quotes, such as for example **„Heme A"**. ***Chemical abbreviations*** of molecular units can be used between curly brackets as in **Fe[C(Si{Me}3)3]2**. Abbreviations recognized by MossWinn are written with bold characters when the stoichiometry is displayed: $Fe[C(Si\mathbf{Me}_3)_3]_2$. The following web site can be consulted concerning already defined abbreviations that can be used: **http://www.mosswinn.hu/abbreviations.htm**. Turn to the corresponding submenu option of the **Help** menu box in the main menu in order to request a new abbreviation code to be used in stoichiometry expressions. Visit the web site **http://www.mosswinn.hu/stsyntax.htm**

for further examples concerning the syntax of stoichiometry expressions.

Press on the stoichiometry edit box with the right mouse button in order

- to set the stoichiometry string to one of the stoichiometry strings of existing own MIDB records, or
- to insert in the stoichiometry string (at the current cursor position) an existing molecular formula abbreviation code.

- **Surface density** - One can give here the total surface density of the measured sample, i.e. the compound mass that was used to prepare the sample divided by the area of the resulting sample (in general the area of the sample's projection on the plane perpendicular to the gamma ray direction). If the value is not available, or it is not applicable, simply leave the field empty.
- **Unit of surface density** - Double-click to toggle between mg/cm^2 and g/cm^2.
- **Temperature [K]** - Sample temperature measured in kelvin (*required field*). If the sample temperature is defined as *room temperature* then write here the approximate sample temperature and include the keyword *RT* in the list of keywords.
- **Isomer shift reference [mm/s]** - One should give here the isomer shift of the IS reference material (characteristic of the current spectrum) relative to that of the standard isomer shift reference material given on the right. The *IS reference material* is defined here as the material that would have an isomer shift of zero on the velocity scale of the current spectrum. For example, if the IS reference material is Fe in Rh matrix at room temperature, then one should write here 0.114 because 0.114 mm/s is the isomer shift of Fe in Rh matrix relative to Fe in bcc iron at room temperature.
- **Standard isomer shift reference for the current source** - This label shows the standard isomer shift reference material that serves as the point of reference for isomer shift values in the database. For this purpose the following standards (standard matrices and temperatures) have been chosen:
  - ^{57}**Fe** - bcc iron , *T*=R
  - ^{119}**Sn** - $BaSnO_3$, *T*=R
  - ^{125}**Te** - Mg_3TeO_6 , *T*=R
  - ^{151}**Eu** - EuF_3 , *T*=R
  - ^{161}**Dy** - DyF_3 , *T*=R
  - ^{121}**Sb** - $CaSnO_3$, 4.2K
  - ^{129}**I** - ZnTe , 4.2K
  - ^{141}**Pr** - PrF_3 , 4.2K
  - ^{237}**Np** - $NpAl_2$, 4.2K
  - ^{197}**Au** - Au metal, 4.2K

In order to be able to give the correct isomer shift reference value in the preceding edit box, it is essential that one knows what the isomer shift of the corresponding standard isomer shift reference material (as given above) would be on the velocity scale of the current spectrum. If this isomer shift value is δ_0 mm/s, then one should write the value of its negative, i.e. $-\delta_0$ in the edit box of **Isomer shift reference [mm/s]**.

- **Ext. magn. field [T]** - If an external magnetic field was applied to the sample during the measurement, write the amplitude value of the external field's flux density (given in Tesla) in this edit box. (The given value should be positive.) If there was no external field applied, write here 0 or leave the field empty.
- **Parallel-field button** - Set this button pressed down if there was an external magnetic field applied to the sample during the measurement, and this field was oriented *parallel* to the direction of the gamma ray.
- **Perpendicular-field button** - Set this button pressed down if there was an external magnetic field applied to the sample during the measurement, and this field was oriented *perpendicular* to the direction of the gamma ray.
- **Source matrix / EMS absorber** - One can give here the source matrix (or the absorber material in the case of **EMS** measurements) applied during the measurement.
- **EMS** (checkbox) - check this box in the case of **EMS** measurements, and uncheck it otherwise. The state of this checkbox influences the function of the **Source matrix / EMS absorber** edit box.
- **Year** - Write here the year of publication of the results associated with the present record. (As given on the associated paper.) If the results were not published, write here the year of the measurement.
- **Further attributes & keywords** - Write here keywords and spectrum attributes separated by comma. Right-click for a list of single-word keywords that are frequently used in existing records of the database. It is recommended to use well-known, common abbreviations whenever possible: e.g. **CEMS** instead of Conversion Electron Mossbauer Spectroscopy, **HTSC** instead of High Temperature Superconductor, etc. It is recommended to give here the oxidation state(s) detected on the basis of the spectrum published, e.g. **Fe2+**, **Eu3+** etc. For intermediate oxidation states the following format is recommended: **Fe2+/Fe3+** for an iron oxidation state between 2+ and 3+, and **Eu2+/Eu3+** for an europium oxidation state between 2+ and 3+, etc. In order to indicate the spin state of Mossbauer nuclides, use separate keywords of the form **S=0**, **S=5/2**, **S=2**, etc.
- **Link to the publication reporting about this measurement** - Write here the link pointing to the website from where the paper - published in connection with the measurement to be included in the record - is accessible for subscribers of the corresponding scientific journal. It is recommended to use the **doi link** of the publication whenever possible. A doi (digital object identifier) link is usually given on the publication's

website, e.g. as **doi:10.1016/S0921-4534(99)00562-6**. In such a doi link replace **doi:** with **http://dx.doi.org/** in order to obtain the real link where the doi points to: **http://dx.doi.org/10.1016/S0921-4534(99)00562-6**. (Alternatively, on the paper's website right-click on the doi link and select *Copy Link Location* in order to put the corresponding real link to the clipboard.) The link to the publication reporting about the measurement can be given by using either of the above formats. If a doi link is not available, use an ordinary **http://** link. If the measurement does not have an associated publication, clear this text box or leave it to display **http://dx.doi.org/**.

Additional information - Write here additional information or an internet link pointing to a website containing additional information concerning the measurement associated with the record. This can also be a doi link to another related paper given as in the case of the previous text box, or it can also be a link to your own website where additional information is made available in connection with the measurement. (For example, on such a website one could give a list of further publications dealing with the same - or closely related - material(s), or one could display figures and other supplementary material not included in the original publication.)

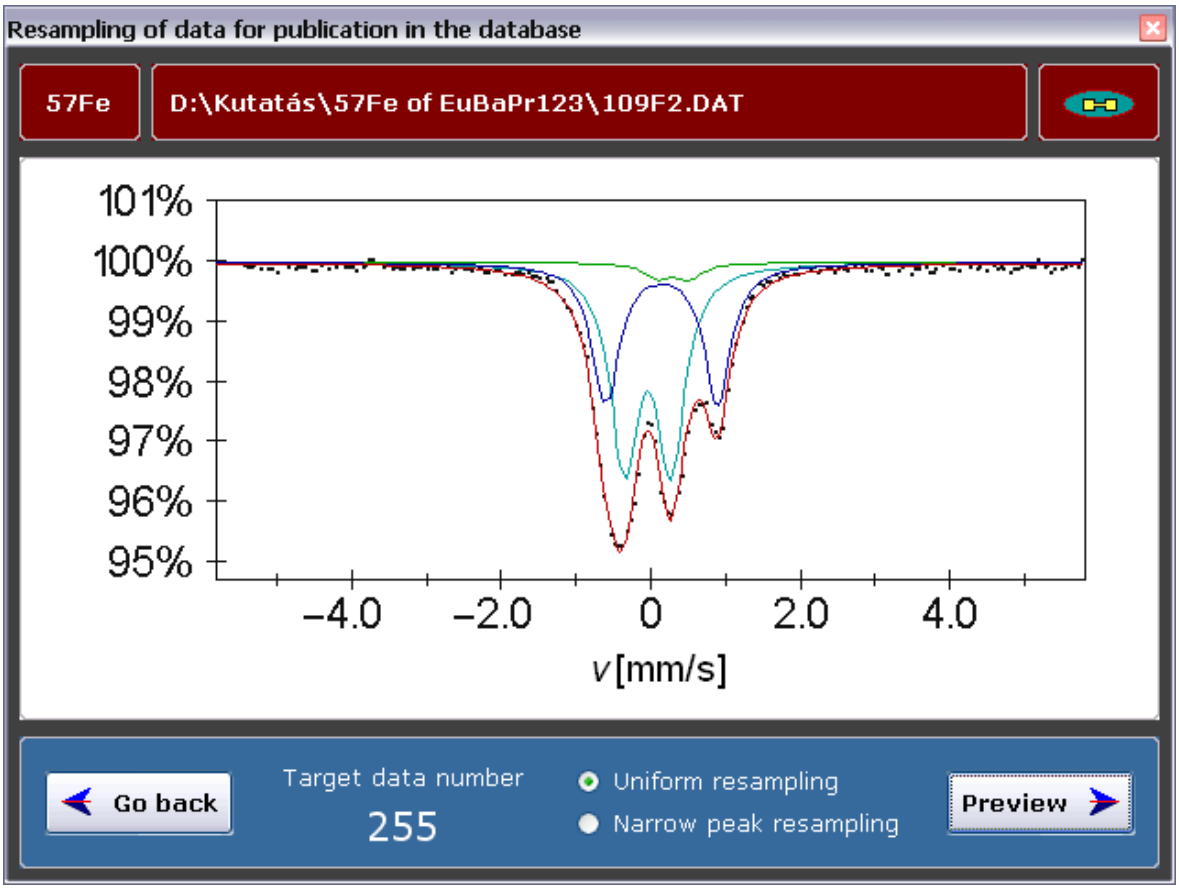
- **Try link** - Press on this button in order to open the associated link in the default internet browser application.
- **Title of publisher** - Write here the title of the researcher who publishes the record (i.e. your title). Use a short version of the appropriate title, e.g. **Mr.**, **Ms.**, **Dr.**, **Prof.** etc., or leave the field empty.
- **Name of publisher** - Write here the name of the researcher who publishes the record (i.e. your name) as **FirstName LastName** (by having at least one space character included before the last name).
- **E-mail of publisher** - Write here the E-mail address of the researcher who publishes the record (i.e. your E-mail address). If the publisher is the corresponding author of the work, then giving the E-mail address will enable interested researchers to contact the corresponding author in connection with the measurement/publication associated with the record.
- **Publisher is corresponding author** - Check this box if the publisher is the corresponding author of the work/measurement associated with the record. If the publisher is not the corresponding author, uncheck this box.
- **First author** - Write here the name of the researcher who authored the work associated with the record as **FirstName LastName** (by having at least one space character included before the last name). If the work/paper was authored by more than one researchers, give here the name of the first author only. If the field is empty, a double-click on it sets the publisher as the first author. Right-click to select the name of the first author from a list of first authors appearing in existing own records.

- **Next** - Press this button in order to proceed to the next form (see page 14) where one can determine whether and how the measured spectrum data and the associated fit model are to be included in the database record.
- **Cancel** - Press this button in order to cancel the publication process and return to the **FIT** menu.

The **MIDB Publisher's Guide** (`http://www.mosswinn.hu/midbguide.htm`) contains further information concerning the publication of MIDB records.

4. Resampling of data for publication

On this form one can determine whether and how the measured spectrum data and the associated fit model are to be included in the database record. In particular, one can set here the number of data points the measured spectrum should be resampled into before being included in the database record.



- **Source nuclide** - Shows the source nuclide that was set in the FIT menu for the current spectrum.
- **Spectrum file** - Shows the path and name of the data file that contains the spectrum associated with the record to be published. (Information on the path and name of the file will not be included in the published record.)
- **Help** - Press on the help ellipse in order to open the corresponding help in the default browser.
- **The resampled spectrum** - Shows the spectrum's resampled (downsampled) form that is going to be published in the database. **In order to exclude/*include* the fitting curve or the measured data from/*into* the published record, press with the right mouse button on the spectrum image, and select the corresponding option.**

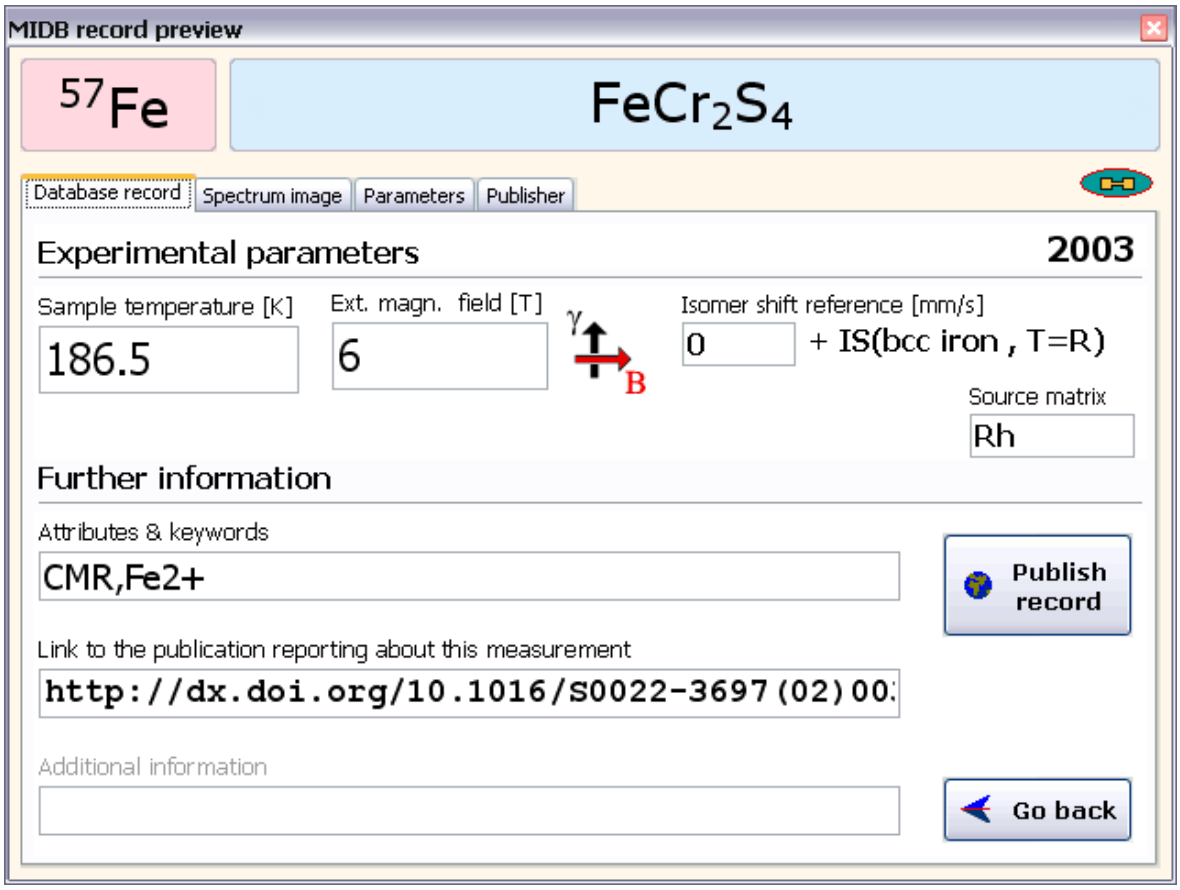
- **Target data number** - Shows the number of data that the spectrum should be resampled into. Press on the data number in order to select another value from a list. The actual data number of the resampled spectrum may be less than the value set here. The data number of the resampled spectrum will always be less than that of the original spectrum, thereby ensuring that the publisher's ownership over the original, full resolution data is not compromised by the act of publication in the database.
- **Uniform resampling / Narrow peak resampling** - Shows the method that is used to prepare the resampled form of the original spectrum. The method of **uniform resampling** tends to sample the original spectrum at equidistant velocity values. Although in most cases uniform resampling will provide optimal results, occasionally it may fail to capture the amplitude of narrow peaks correctly. In such a case select the method of **narrow peak resampling**.
- **Go back** - Press on this button in order to go back to the *database record input form* (see page 7).
- **Preview** - Press on this button in order to proceed to the *database record preview form* (see page 16) that will show how the record will be displayed in the MIDB browser after the publication process is completed.

Note concerning distribution fits

The fitting curve produced via arbitrary-profile distribution fits as carried out by MossWinn is sensitive to the number of data points in the spectrum. As a result, downsampling of the corresponding spectrum may lead to a distribution fitting curve that is different from that fitted to the full resolution spectrum. In such a case try different target data numbers: one of them usually produces a satisfactory result.

5. Database record preview

This form shows how the record will be displayed in the MIDB browser after the publication process is completed. Note that the record's content is displayed on 4 different pages, accessible via the corresponding tabs. See the section on the database browser (page 18) for a detailed account of the meaning of the various items present on this form.

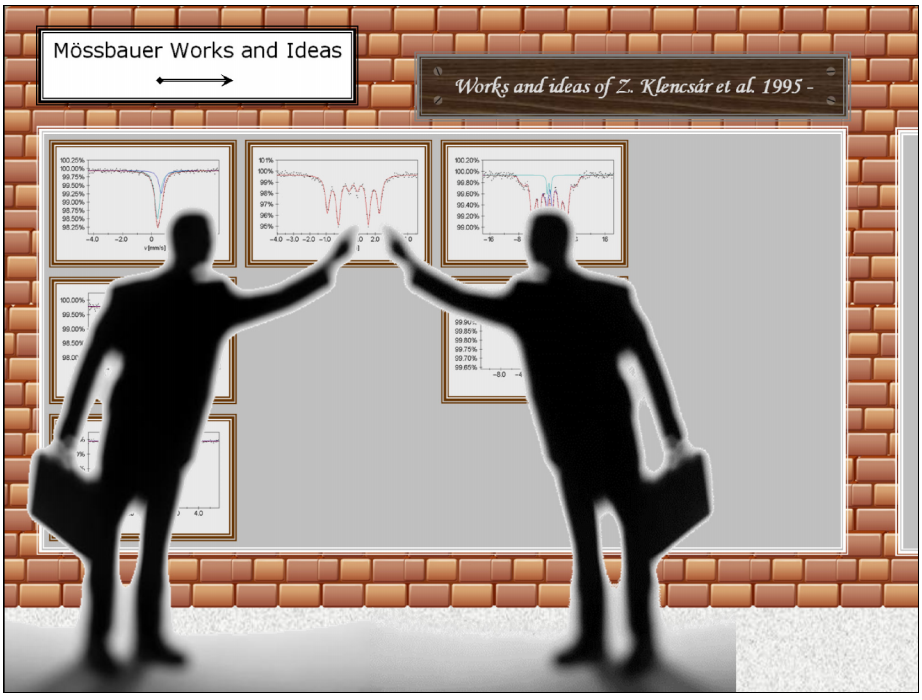


- **Database record** - Press on this tab to inspect the database record card displaying the parameters set previously on the Database record input form (see page 7).
- **Spectrum image** - Press on this tab to inspect the spectrum as it will be displayed in the database browser.
- **Parameters** - Press on this tab to inspect the fit parameters report as it will be displayed in the database browser.
- **Publisher** - Press on this tab to inspect the settings concerning the name and E-mail of the publisher and whether the publisher is the corresponding author of the present record.
- **Go back** - Press on this button in order to return to the previous (Resampling of data, see page 14) form.

- **Publish record** - Press on this button in order to publish the database record in the MossWinn Internet Database. After successful publication the record becomes ready to appear in the MIDB browser of database subscribers all around the world. If you want to edit or withdraw a published record, turn to the corresponding option of the DB menu (see page 4).

Note concerning your control over the published database records

Even though the publication of a database record necessitates the sending of the file associated with the record over the internet to the database server, from where it can then be downloaded onto the computer of MossWinn licensees all around the world, unlike in the case of usual databases **you do not lose direct control over your published data**. Namely, you can edit/withdraw your record by the help of the corresponding menu option of the DB menu any time, which action will update/remove the corresponding record on/from the database server as well as all the computers onto which the record was downloaded from the database server (the local copies of MossWinn take care of this latter action during synchronization events). This means that in effect **the MossWinn Internet Database rather functions as a display window to your scientific achievements**, which window you can open / rearrange / enlarge / reduce / close any time you want to. Withdrawal of your existing own database records is possible even in the absence of an active subscription to the database service.



Publishing records in the MossWinn Internet Database is
like opening a display window to your scientific achievements.

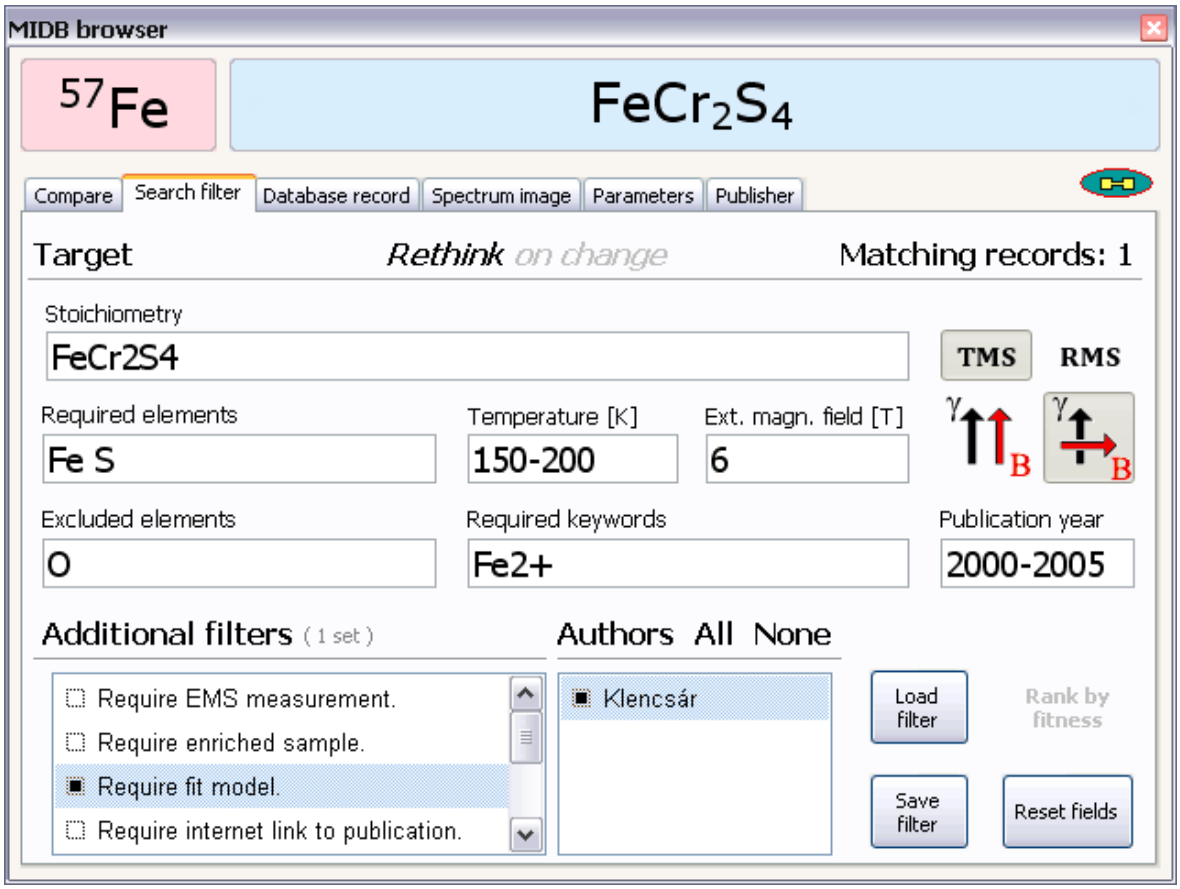
6. The database browser

In order to browse the records included in the database enter the **FIT** menu, press on the **DB** menu box and select the option **Browse the internet database**. As a result, the **MIDB browser** form becomes displayed, which enables one

- to search database records according to various criteria,
- to inspect, copy, print (downsampled) spectra and associated fitting curves included in MIDB records,
- to inspect, copy, print detailed fit reports associated with MIDB records,
- to place reprint requests for articles associated with MIDB records, and
- to compare and apply fit models, included in MIDB records, to one's own spectrum.

The **MIDB browser** form contains a headline and several tabs which functions are explained below.

- **Source nuclide** - In the search process the database browser considers only those records that are associated with Mossbauer measurements carried out by the help of the source nuclide shown in this (pink) menu box. Press on the menu box in order to select another source nuclide from the appearing popup list.



- **Stoichiometry** - Displays the stoichiometry of the material associated with the record that (1) was either returned by the search as the best match to the currently set criteria or (2) was selected by the user from a list of records returned by the search. In order to access the list of returned records, press on the (sky blue) stoichiometry box. In the appearing popup the records are listed in descending order of their fitness to the current search criteria, the topmost record being the best match. The list of returned records informs about the number of subspectra contributing to the fit model of a particular record in the form of **S***n* where *n* is the number of subspectra. If one or more of the subspectra is subject to a distribution (e.g. hyperfine magnetic field distribution), then the character **D** is added to the notation: **S***n***D**. *Right-click* on the stoichiometry box in order to access one of the following options:
  - **Copy to clipboard as plain text** - Select this option in order to copy the stoichiometry string into the clipboard as plain text, without any formatting.
  - **Copy to clipboard as RTF text** - Select this option in order to copy the stoichiometry string into the clipboard as RTF text, with the subscripts and superscripts preserved as lowered and raised characters, respectively.
  - **Copy to clipboard as HTML text** - Select this option in order to copy the stoichiometry string into the clipboard as HTML code (plain text) ready to be pasted into the code of a HTML page.
  - **Copy to clipboard as source code** - Select this option in order to copy the stoichiometry string into the clipboard as the corresponding — plain text — source code on which the displayed formatted stoichiometry is based.
  - **Copy to clipboard as image** - Select this option in order to copy the stoichiometry string into the clipboard as a monochrome bitmap image.
  - **Look up abbreviations** - Select this option in order to access information concerning molecular formula abbreviations being part of the shown stoichiometry string. The abbreviations in question are listed as submenu options that can be selected to open a web page with corresponding information in the default browser. (The option is available only when the stoichiometry includes an abbreviation code.)

Search filter page

- **Help** - Press on the help ellipse in order to open the corresponding help in the default browser.
- ***Rethink*** (button) - Press on this button in order to execute the database query according to the current search criteria. As a result, the stoichiometry menu box will be updated to display the sample stoichiometry associated with the record that is evaluated to be the best match to the current criteria. The list of returned records becomes updated, too. When the *on change* flag is set, rethink is carried out automatically whenever the search criteria change.
- ***on change*** (flag) - Press on this flag to toggle between manual and automatic rethink modes. When the flag is not set (the ***on change*** text being grayed out as on the figure above), then the database search has to be initiated manually by a press on the ***Rethink*** button. When the flag is set (the ***on change*** text being displayed in black), then the database search / query is repeated automatically whenever the search criteria change. The latter option is more convenient when the search process is

fast, whereas the former option is recommended when the search process turns out to be slow (e.g. when the **Rank by fitness** mode has been initiated).

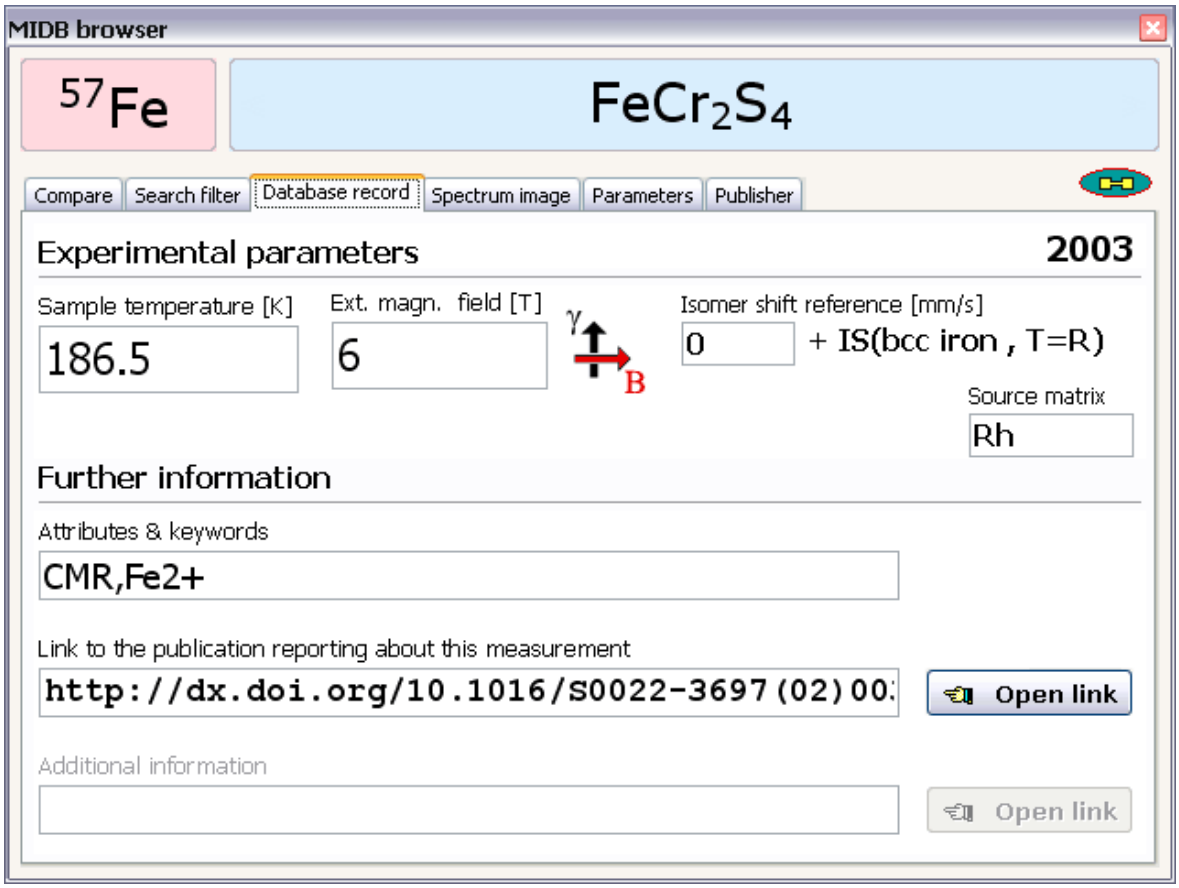
- **Matching records** - Shows the number of records matching the search criteria for which the last database query was executed. The list of returned records shows only the best of the matching records.
- **TMS** - Press this button down in order to search *exclusively* for those records that are associated with *transmission type Mossbauer spectroscopy* measurements. When the button is in the down state, press on it in order to change it back to the up state.
- **RMS** - Press this button down in order to search *exclusively* for those records that are associated with *reflection type Mossbauer spectroscopy* measurements (e.g. CEMS). When the button is in the down state, press on it in order to change it back to the up state.
- **Stoichiometry** - Set here the stoichiometry of the compound that you want to query the database for. One can use here the same textual format as on the Database Record Input Form (see page 7). While the query will consider the stoichiometry set here as the desired stoichiometry, it may also return records that are associated with compounds having a different stoichiometry.
- **Required elements** - List here the symbol of elements (separated by comma or space) that are required to be present in the compounds associated with the records returned by the database query. This is an effective way to narrow down database searches.
- **Excluded elements** - List here the symbol of elements (separated by comma or space) that are not allowed to be present in the compounds associated with the records returned by the database query. This is an effective way to narrow down database searches.
- **Required keywords** - List here the keywords (separated by comma) that are *all* required to be associated with the records returned by the database query. Right-click for a list of keywords associated with existing records of the database.
- **Temperature [K]** - Write here the target measurement temperature or a target measurement temperature interval (e.g. **100-180**) for the records searched for. If a single temperature value is given, then queries will consider the temperature in question as the desired temperature but may also return records associated with measurements carried out at a different temperature. If a temperature interval is given, then records — associated with measurements carried out at a temperature — outside this interval will not be returned. (The interval is treated as a closed interval.)
- **Ext. magn. field [T]** - Write here the target external magnetic field (*emf*) or a target emf interval (e.g. **3.5-6.5**) for the records searched for. If a single emf value is given, then queries will consider the emf in question as the desired emf but may also return records associated with measurements carried out in a different external magnetic field. If an

emf interval is given, then records — associated with measurements carried out in an external magnetic field — outside this interval will not be returned. (The interval is treated as a closed interval.)

- **Parallel field button** - Press this button down in order to search *exclusively* for those records that are associated with measurements that were carried out by applying an external magnetic field whose direction was **parallel to** that of **the gamma ray**. When the button is in the down state, press on it in order to change it back to the up state.
- **Perpendicular field button** - Press this button down in order to search *exclusively* for those records that are associated with measurements that were carried out by applying an external magnetic field whose direction was **perpendicular to** that of **the gamma ray**. When the button is in the down state, press on it in order to change it back to the up state.
- **Publication year** - Write here the target publication year or a target publication year interval (e.g. **1997-2003**) for the records searched for. If a single year value is given, then queries will consider the year in question as the desired publication/measurement year but may also return records associated with a different publication/measurement year value. If a year interval is given, then records associated with publication/measurement year values outside this interval will not be returned. (The interval is treated as a closed interval.)
- **Additional filters** - Select here additional filters in order to narrow down the database search accordingly. The list box offers the following options:
  - **Require EMS measurement** - When selected, database queries return only records associated with EMS (emission Mossbauer spectroscopy) measurements.
  - **Require enriched sample** - When selected, database queries return only records associated with a sample stoichiometry that contains the symbol of Mossbauer nuclide with the mass number explicitly written out indicating a sample that is enriched in the isotope in question (e.g. $Eu(Ba_{1.3}Pr_{0.7})(Cu_{0.99}{}^{57}Fe_{0.01})_3O_7$).
  - **Require fit model** - When selected, database queries return only records that contain a fit model.
  - **Require internet link to publication** - When selected, database queries return only records that contain an internet link to an associated publication.
  - **Require measured data** - When selected, database queries return only records that contain measured data in the form of a downsampled spectrum.
  - **Require own record** - When selected, database queries return only own records, i.e. records that were published by having the same hardware key attached to the computer.
  - **Require publisher to be the author** - When selected, database queries return only records that were published by the corresponding author.
  - **Require single-phase compound** - When selected, database queries return only records that are associated with single-phase compounds, i.e. compounds whose stoichiometry string does not contain the **+** character.
- **Authors** (list box) - The authors' list box displays the surname of authors who appear as first author in one or more of the published records associated with the selected source nuclide. Database queries consider only those records that are associated with first authors whose surname is selected here.

- **Authors** (title) - Press on this title in order to select/deselect one of the author surnames (listed in the authors' list box) in the appearing popup list. If one or more of the author surnames is not selected in the authors' listbox, then the **Author** title appears as here, i.e. grayed out.
- **All** (button) - Press on this button in order to select all author surnames in the authors' list box.
- **None** (button) - Press on this button in order to deselect all author surnames in the authors' list box.
- **Load filter** (button) - Press on this button in order to load a previously saved filter set. This will overwrite all fields on the Search filter page.
- **Save filter** (button) - Press on this button in order to save all the fields on the Search filter page in a filter set file. The file thus saved, and the associated filter settings, can be loaded back via the Load filter button.
- **Reset fields** (button) - Press on this button in order to reset all the fields on the Search filter page to their default value as determined by the attributes of the spectrum under study in the FIT menu.
- **Rank by fitness** (button) - Press this button down in order to have returned database records sorted according to their fitness to the measured spectrum data that is under study in the fit menu. When this button is down, then the *Stoichiometry*, *Temperature [K]*, *Ext. magn. field [T]* and *Publication year* edit boxes are disabled, and their content is not considered while a database query is executed. The fitness of the records is evaluated by comparing the measured data (or the fit model in the absence of measured data) included in the records with the counts data of the measured spectrum under study. This is a rather computation-intensive comparison process that may result in slow execution of database queries. Therefore, **before the rank by fitness comparison mode is selected, it is recommended to disable the automatic *Rethink on change* function**. The same comparison/ranking method is used when the **Find and apply best match** menu option of the **DB** menu is selected directly in the **FIT** menu.

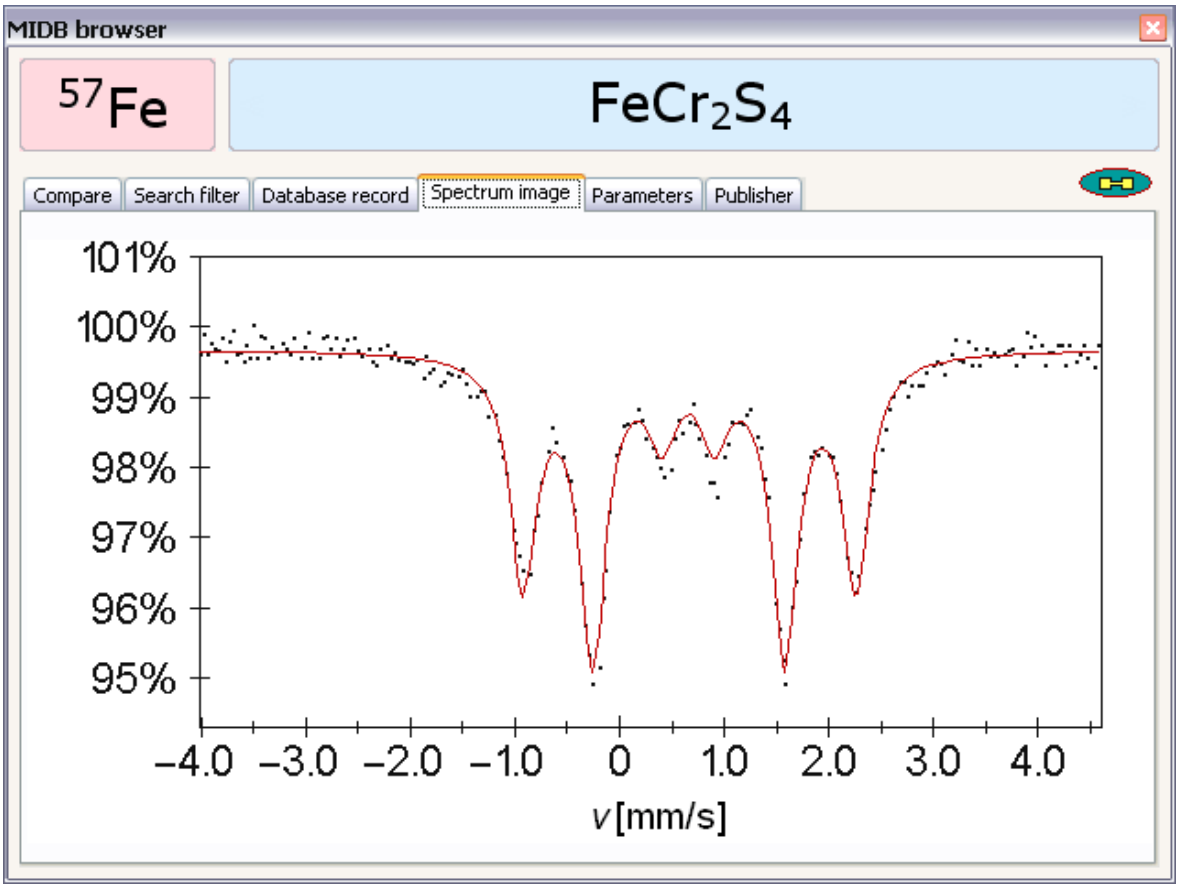
Database record page



- **Help** - Press on the help ellipse in order to open the corresponding help in the default browser.
- **Publication year** - Publication year of the article associated with the record, or the year of measurement in the absence of a corresponding publication.
- **Temperature** - Temperature of the sample during the measurement.
- **External magnetic field** - Flux density of the external magnetic field applied to the sample during the measurement.
- **Orientation of the external magnetic field** - Shows the orientation of the external magnetic field (parallel or perpendicular) with respect to the direction of the gamma ray.
- **Isomer shift reference** - Isomer shift of the isomer shift reference material (being a characteristic of the velocity scale of the measured spectrum associated with the record) with respect to the standard given on the right.
- **Source matrix** - Shows the matrix material of the applied radioactive source, or the absorber material in the case of EMS measurements.
- **Attributes & keywords** - Shows the comma-delimited keywords and attributes associated with the record.

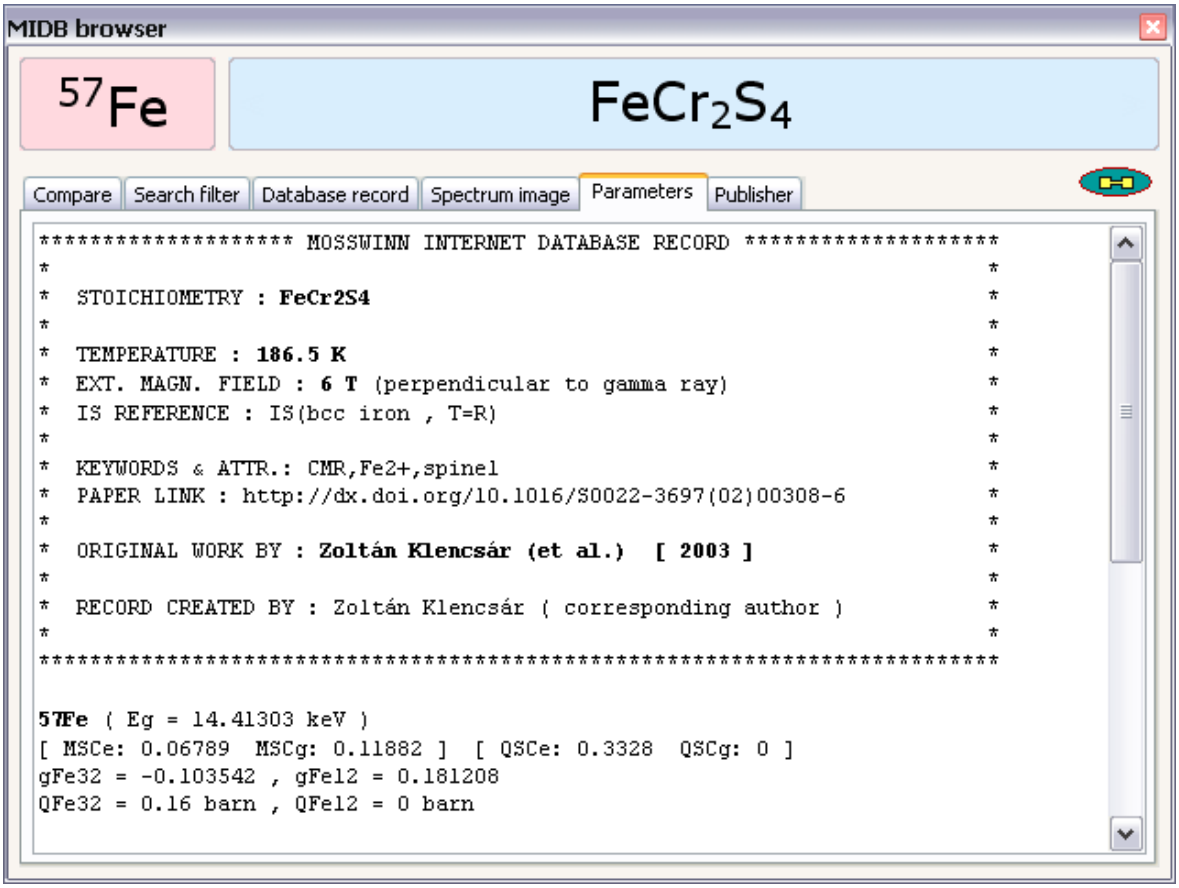
- **Link to the publication reporting about this measurement** - Internet link to the website of the article published about the measurement.
- **Additional information** - Additional textual information, or internet link to a website displaying additional information concerning the record.
- **Open link** - Press this button in order to open the corresponding link in the default browser.

Spectrum image page



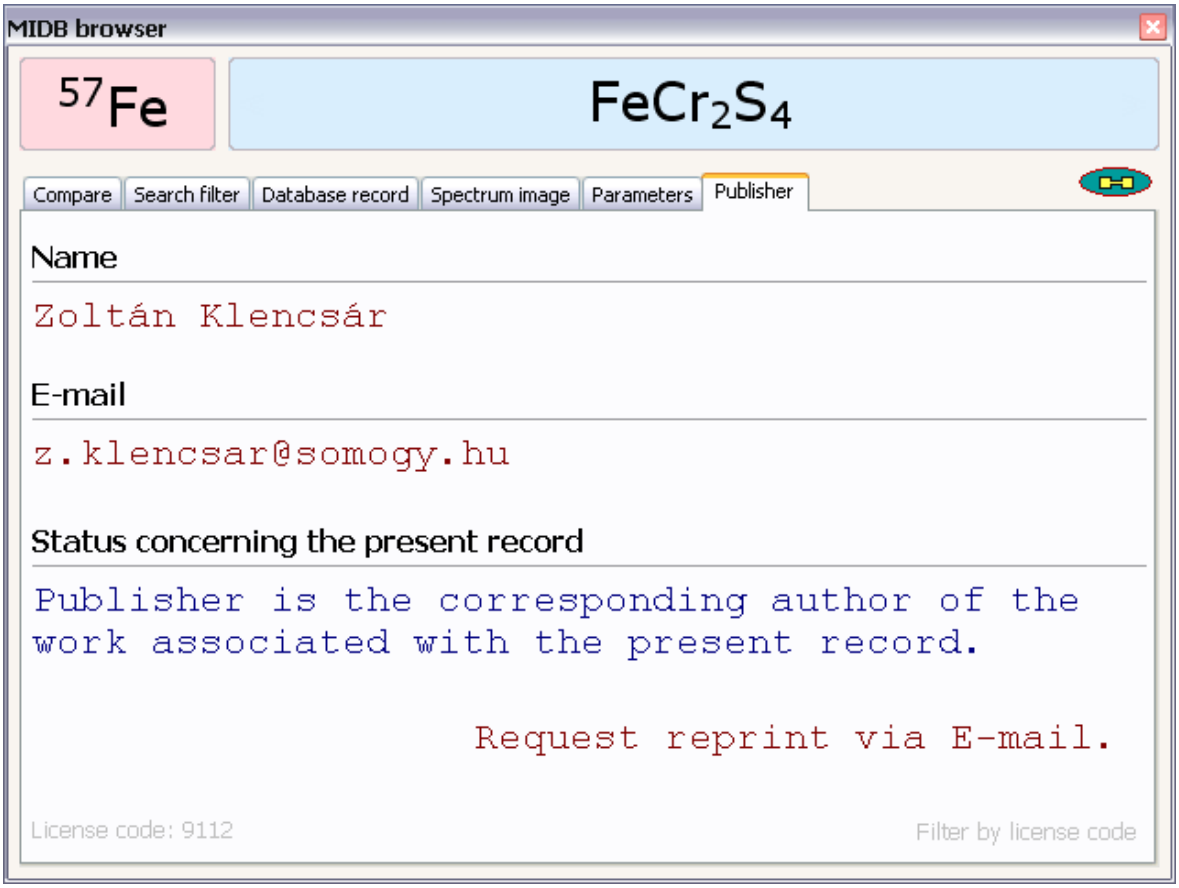
- **Help** - Press on the help ellipse in order to open the corresponding help in the default browser.
- **Spectrum image** - Shows the downsampled version of the measured spectrum and the fitting curve calculated on the user's PC on the basis of the fit model and nuclear constants included in the shown record, which latter may be different from the nuclear constants currently in effect on the user's PC. *Right-click* on the image in order to access the following options:
  - **Copy to clipboard** - Select this option in order to copy the shown spectrum image to the clipboard of Windows. The resolution of the copied image is fixed to 614×330 pixels.
  - **Print to printer** - Select this option in order to print the shown spectrum image to the default printer.

Parameters page



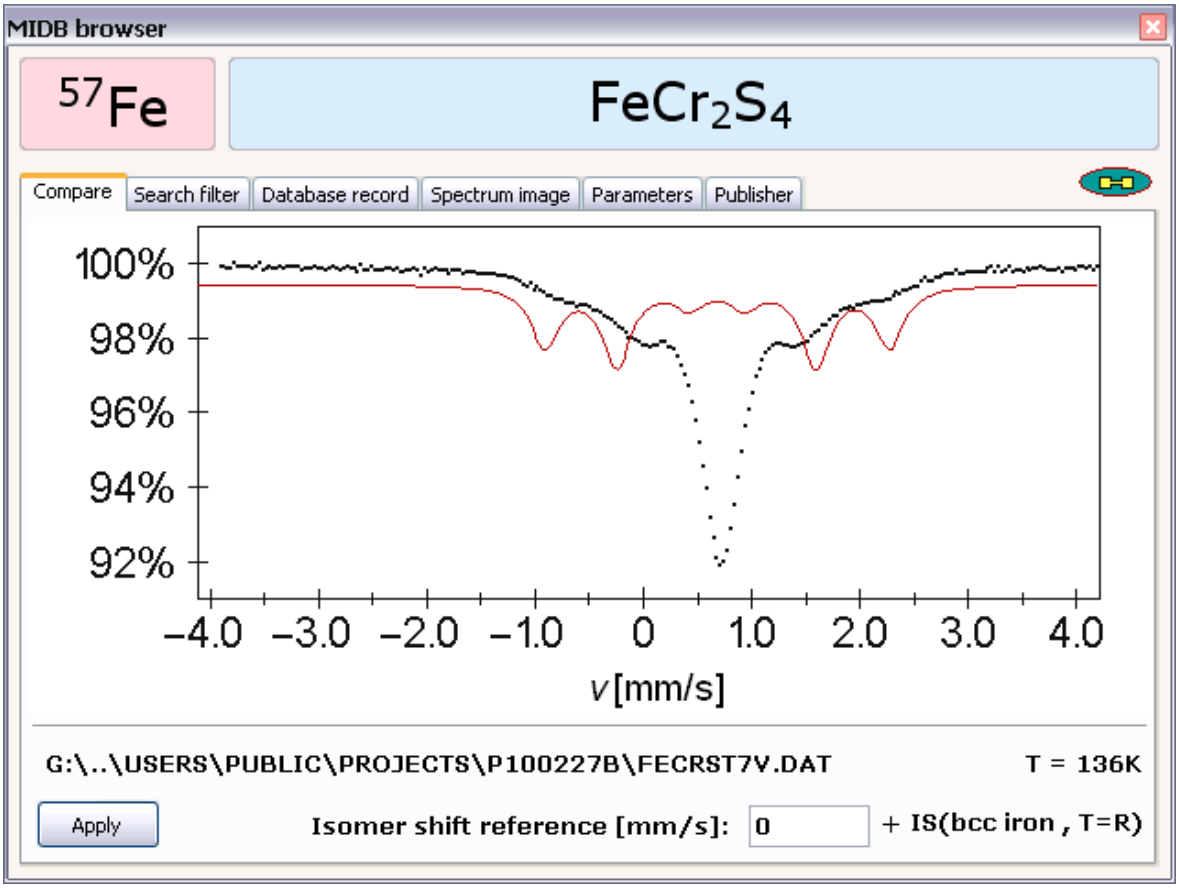
- **Help** - Press on the help ellipse in order to open the corresponding help in the default browser.
- **Parameters / Fit report** - Shows the parameters and fit report associated with the record. The value of nuclear parameters used on the publisher's PC when the record was created are shown as well (see the manual for the meaning of the applied abbreviations). *Right-click* on the image in order to access the following options:
  - **Copy to clipboard** - Select this option in order to copy the parameters / fit report to the clipboard of Windows.
  - **Print to printer** - Select this option in order to print the parameters / fit report to the default printer.

Publisher page



- **Help** - Press on the help ellipse in order to open the corresponding help in the default browser.
- **Name of the publisher** - Shows the name that was given, by the researcher who published the record, as the name of the publisher.
- **E-mail of the publisher** - Shows the E-mail address of the publisher. Press on it in order to open an E-mail, addressed to the given E-mail address, in the default E-mail client.
- **Request reprint via E-mail.** - Press on this text in order to open an automatically written reprint request E-mail (concerning the shown record) in the default E-mail client.
- **License code** - The unique license code identifies the MossWinn license hardware key that was attached to the publisher's PC when the displayed record was published.
- **Filter by license code** - Press on this button in order to filter records by the unique license code associated with them. The corresponding filter, set on the appearing form, will be preserved even if MossWinn is restarted. When filtering records by license code, consider that a single license code may be associated with several publishers (e.g. several researchers using the same copy of MossWinn) as well as with several different authors. The license code filter is effective only on the local system on which it is set.

Compare page

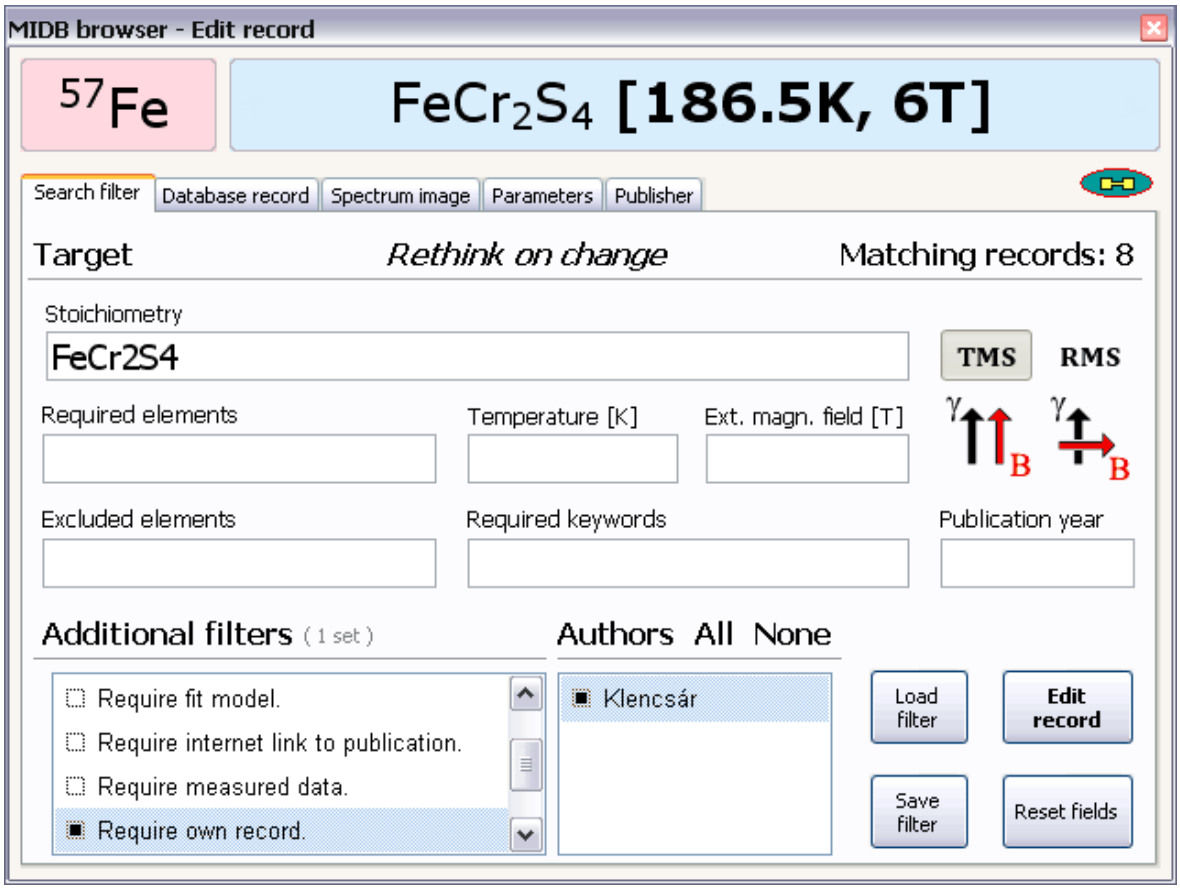


- **Help** - Press on the help ellipse in order to open the corresponding help in the default browser.
- **Own spectrum compared to the fit model included in the record** - Shows the own spectrum (displayed also in the FIT menu) as being compared to the fit model of the record.
- **File name and path of the fitted spectrum** - This is the name and path of the fitted spectrum.
- **Parameters of the fitted spectrum** - Temperature (and external magnetic field, if applicable) characteristic to the fitted spectrum. (Not to be confused with the corresponding parameters characteristic to the selected record.)
- **Isomer shift reference characteristic to the fitted spectrum** - See page 10 for details.
- **Apply** (button) - Press on this button in order to apply the shown (red curve) fit model — taken from the database record — to the fitted spectrum (scatter graph), and return to the FIT menu.

7. How to edit database records

- In order to **edit** a record published in the MIDB database, select the **Edit record published in the internet database** submenu of the **DB** menu box in the **FIT** menu. As a result, the MIDB browser form appears with the additional button displaying **Edit record** (see image below). The own record that is to be edited in the database can be selected by the help of the MIDB browser. Once the record is selected, press on the **Edit record** button in order to open the **Database record input form** (see page 7) with the corresponding record parameters available for editing. One can edit only those parameters of the record that are displayed on this form, i.e. the editing of the resampled spectrum data and that of the fit model is not possible. (In order to change the latter data, the record needs to be withdrawn and then republished in the form of a newly created record.)

  Alternatively, to edit database records one can also turn to the corresponding submenu option of the **DTB** menu box in the main menu.



8. How to withdraw database records

- In order to **withdraw** a record from the MIDB database, select the **Withdraw record from the internet database** submenu of the **DB** menu box in the FIT menu. As a result, the MIDB browser form appears with the additional button displaying **Withdraw record** (see image below). The own record that is to be withdrawn from the database can be selected by the help of the MIDB browser. Once the record is selected, press on the **Withdraw record** button in order to withdraw the selected record from the database.

  Alternatively, to withdraw database records one can also turn to the corresponding submenu option of the **DTB** menu box in the main menu.