The new WEB-accessible online database of the Mössbauer effect data center

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Abstract

The web-accessible online database (WAD) of the Mössbauer Effect Data Center (MEDC) is one of the worldwide available information services provided by MEDC to the scientific community. It is based on the uniquely wide scope Mössbauer spectroscopy database that has been compiled and maintained by MEDC since the 1960's. Following enhancements applied to the capabilities of the MEDC core database in connection with the development of a new database management software named "MEDC DBM", the development of a new web-accessible online database (MEDC WAD) was started in 2019. Here we introduce the current state and the main features of the newly developed MEDC WAD system with emphasis put on its novel and rather unique attributes that can effectively aid the scientific research process in the field of Mössbauer spectroscopy.

Keywords Mössbauer effect data center · Database · Mössbauer spectroscopy · Information service · New management software

1 Introduction

The web-accessible online database (WAD) of the Mössbauer Effect Data Center (MEDC) is based on the uniquely wide scope Mössbauer spectroscopy database that has been compiled and maintained by MEDC since the 1960's [1–7]. In order to further increase the added value of the MEDC database to the scientific research process, a further development of the database has been recently started [7, 8]. The capabilities of the MEDC core database (that currently

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includes bibliographical details of above 62,000 Mössbauer spectroscopy related publications, along with above 117,000 associated data records) were improved first via the development of a new database management software named "MEDC DBM" [8] and via associated enhancements applied to the database structure. In particular, as part of the latter, fields capable of storing the DOI link [9] of publications and the hyperfine/apparent magnetic field value of magnetic spectral patterns have been added to the database structure.

The MEDC database infrastructure has been built in such a way that the data required by the various database-related information services (such as the issues of the Mössbauer Effect Reference and Data Journal [10] as well as the web-accessible online Mössbauer database [6, 11]) need to be provided by the database management software [8], the latter maintaining the original and most detailed version of the database data compiled by the database editors. This approach has the advantage that the different services derived from the same detailed core database may be tailored to their specific purpose, thereby making them more focused and potentially more useful to researchers. In addition, quasi automatic derivation of the services' data from the MEDC core database can provide the services with the necessary flexibility required by the incorporation of new functionalities made eventually possible by further developments of the core database.

In particular, the functions and query possibilities that can be offered by the web accessible online database are determined mainly by the structure and data of the MEDC core database. The WAD that makes MEDC database data accessible to researchers can be seen as being composed of mainly two fundamental constituents (Fig. 1). One is the WAD's underlying data and data structure (the regularly updated database tables, along with their fields and associated relations) that are essentially produced by the MEDC DBM database manager software when it outputs the data for WAD in the form of an SQL file representing the regularly updated content of the WAD. The second is the web-based user interface system (UIS) that allows researchers to query the database. These two constituents need certainly be developed in unison with each other. In addition, as a third component, the WAD may also contain data
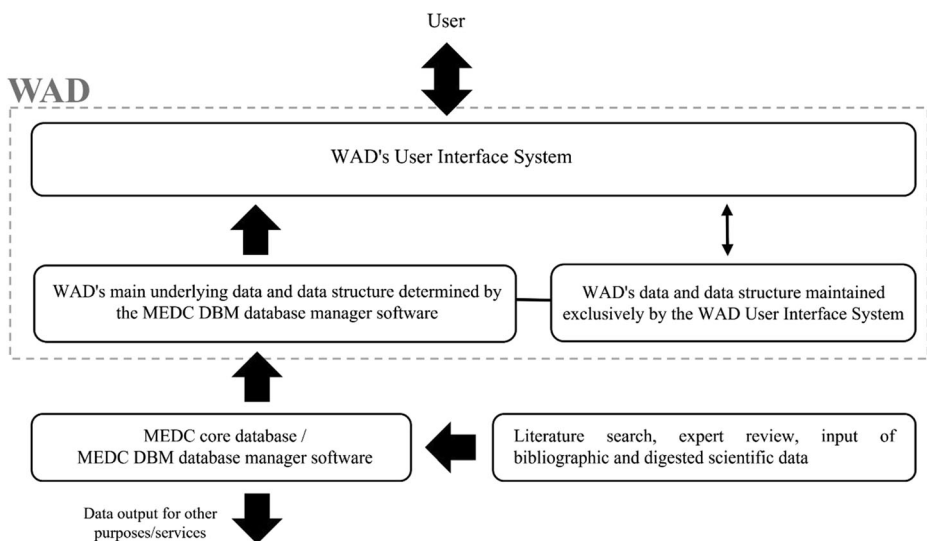

Fig. 1 Schematic chart of the flow of MEDC database data in relation with the web-accessible online database (WAD) emphasizing the structure and components of the latter

tables (including, e.g., users' favorite query settings, notes and marked list of references, see further on) that are neither output by the database manager software nor are regularly updated, but are rather managed exclusively via the WAD UIS.

The previous version(s) of MEDC's WAD have been available now for ca. two decades [6, 11]. Its data with the required structure can be generated by the MEDC DBM software, and consequently this older WAD system is still available through MEDC's website [6]. Instead of improving the previous system, in order to achieve progress in this field, a completely new WAD system has been developed during the years 2019–2020, which operates independently from its predecessor and is already accessible through MEDC's website [6] as well. In the present work we introduce the main characteristics and the main novel functions of this newly developed system.

2 Novel functions of the new WAD system

Concerning its technical realization the new WAD system is based on building blocks similar to those of the earlier one: data are stored in the form of a MySQL relational database, server-side programming and the database connection are realized via PHP scripts (in its current version compatible with PHP version 5.3.6) producing the query outputs as HTML documents suitable to be displayed by the clients' web browser. User interactions and dynamic effects on the client side are handled by web forms, CSS (cascading style sheets) and JavaScript. The design of the user interface (Fig. 2) is based on a customizable website template [12].

With respect to the older system, the new WAD handles database queries and presents query results in an improved manner: as opposed to querying only a single table (such as, e.g., "References" or "Data") selected at the beginning of the database query process, one can now

Fig. 2 Snapshot of the screen of the new WAD system as it is displayed in a web browser after a database query has been executed returning 19 reference matches, along with a few added notes identifying the displayed menus and visual elements. See text for details

combine query criteria related to bibliographic and Mössbauer data arbitrarily, and it remains the job of the server side PHP script to decide which database table(s) to turn to in order to check the fullfillment of the query criteria and which table(s) to look up in order to return the appropriate results. While previously the returned results were limited to the information (e.g. bibliographic details without Mössbauer parameter datasets in the case of the "References" table or Mössbauer parameter datasets without detailed bibliographic information in the case of the "Data" table) available in the specific table that was queried, in the new WAD bibliographic information (in the following: references) and the associated Mössbauer datasets are always returned together as query answers. The user is then offered several options to visualize the returned query results (Fig. 3), and may decide to survey.

(a)   the returned references together with their associated Mössbauer datasets,
(b)   the returned references separately without the associated Mössbauer datasets,
(c)   all the Mössbauer datasets associated with the returned references,
(d)   all the Mössbauer datasets (associated with the returned references) that match the query criteria set for the datasets (if any was defined).

As indicated on Fig. 3a, via the local menu system (appearing when the mouse is moved over the menu symbol ≡) the returned references may be marked to build a list of marked references that can then be invoked and displayed together later on. Furthermore, one may also search for further references where either the measured absorbers contain a similar set of chemical elements or the reference is associated with similar keywords as those characterizing the selected reference. In addition, database editors and users who are the coauthors of the selected work also have the possibility to add and view notes associated with the reference in question. The latter establishes an interactivity channel between the users/authors and the editors, thereby promoting author feedback related to the database records and consequently also the correction of errors in the records should there be any discovered. Users may also have the possibility to list, review and add a note to all records dealing with publications that the user is a coauthor of. Own notes can be edited and deleted as well.

Conditions that can be combined in order to set up database queries are organized into several groups as listed in Table 1. In order to be returned as matching answer to a query, references must satisfy all the set conditions, except where the condition explicitly refers to the exclusion of references satisfying the condition. References satisfy the conditions associated with Mössbauer parameter data sets if they have at least one data set that satisfies the conditions.

When the query is submitted, a PHP script interprets and translates it to a database SQL Select statement that is subsequently displayed together with the returned results (Fig. 4), which allows one to monitor the query translation process. Internally, however, the PHP script may retrieve the query results in an alternative (but compatible) way that leads essentially to the same results as the displayed Select statement would.

If a query produced results associated with references published in multiple scientific journals, then the *Journal filter* condition group becomes available (Fig. 2), which offers the possibility to apply further filters regarding the name of the journals in question.

Beside the condition groups listed in Table 1, queries may also be issued via free text entered in a search box (Fig. 2). Internally the entered text is interpreted as a space-separated list of words. The individual words are then analyzed by the PHP script for their possible

1 reference match

(a)

| 84D015 | J.W.C.De Vries*, R.C.Thiel, K.H.J.Buschow, *Physica B+C (Amsterdam)* **124B** (1984) 291-8 | | | | | ENG | 0700 | ≡ |

| 151Eu | The 151Eu Mossbauer Isomer Shift in Intermetallic Compounds Containing Trivalent Europium | | | | | Mark reference | | |

Isotope	T_s	T_a	Source	Absorber	IS, mm/s	QS, mm/s	MF, T	Comments
151Eu		R	SmF3(IS/EuF3)	EuIr$_2$	1.76		Find articles related by elements	anomalous behavior, val
151Eu		R	SmF3(IS/EuF3)	EuNi$_5$	2.3		Find articles related by keywords	anomalous behavior, val
151Eu		R	SmF3(IS/EuF3)	EuPd$_3$	4.23		Add note	anomalous behavior, valence instabilities
151Eu		R	SmF3(IS/EuF3)	Eu$_2$Ni$_{17}$	2.45			anomalous behavior, valence instabilities

1 reference match

(b)

[84D015] J.W.C.De Vries, R.C.Thiel, K.H.J.Buschow, **The 151Eu Mossbauer Isomer Shift in Intermetallic Compounds Containing Trivalent Europium**, *Physica B+C (Amsterdam)* **124B** (1984) 291-8.

All data of 1 reference match

(c)

Reference	Isotope	T_s	T_a	Source	Absorber	IS, mm/s	QS, mm/s	MF, T	Comments
84D015	151Eu		R	SmF3(IS/EuF3)	EuIr$_2$	1.76			anomalous behavior, valence instabilities
84D015	151Eu		R	SmF3(IS/EuF3)	EuNi$_5$	2.3			anomalous behavior, valence instabilities
84D015	151Eu		R	SmF3(IS/EuF3)	EuPd$_3$	4.23			anomalous behavior, valence instabilities
84D015	151Eu		R	SmF3(IS/EuF3)	Eu$_2$Ni$_{17}$	2.45			anomalous behavior, valence instabilities

Matching data of 1 reference match

(d)

Reference	Isotope	T_s	T_a	Source	Absorber	IS, mm/s	QS, mm/s	MF, T	Comments
84D015	151Eu		R	SmF3(IS/EuF3)	EuNi$_5$	2.3			anomalous behavior, valence instabilities
84D015	151Eu		R	SmF3(IS/EuF3)	Eu$_2$Ni$_{17}$	2.45			anomalous behavior, valence instabilities

Fig. 3 Different alternative visualizations of the same query result as returned by the new WAD system as response to the query requesting ^{151}Eu Mössbauer results published in 1984, where the standard ^{151}Eu isomer shift (i.e. a value meant wrt. EuF$_3$ at room temperature) obtained is inside the range of 2...3 mm s^{-1}. From top to bottom: (a) the returned reference together with its associated Mössbauer datasets and additional options indicated (editorial view), (b) the returned reference separately without the associated Mössbauer datasets, (c) all the Mössbauer datasets associated with the returned references with non-matching datasets grayed out, and (d) all the returned reference's Mössbauer datasets that match the query criteria

meaning, i.e. whether they denote an author name, a keyword code, a publication year, a journal name or other type of information. The database query is then issued on the basis of the result of this analysis. Whether the latter was successful in interpreting the user's intention may be checked on the returned SQL Select statement. For example, the text *71M022 Mossbauer Wagner IR3 FE7 Ni MAA 1970–1980 "Phys. Chem." v26 p343 "Nuclear Gamma"* when entered into the search box and submitted as query (by pressing on the search icon $\mathcal{P}$), results in the SQL Select statement shown in Fig. 5, and returns the reference [71M022] R.L. Mössbauer, M.Lengsfeld, W.Von Lieres, W.Potzel, P.Teschner, F.E.Wagner, G.Kaindl, Nuclear Gamma Resonance Study of the Ir-Fe and Ir-Ni Alloy Systems, *Z. Naturforsch., A: Astrophys., Phys. Phys. Chem.* **26** (1971) 343.

Table 1 Condition groups and their associated conditions with corresponding value types given between parentheses. Selectors offer a predefined list of options. When a list of words is required, then all the given words must be present in the corresponding field in order to have the condition satisfied. When exclusion is based on a list of words, then all the given words must be absent in the corresponding field in order to avoid exclusion from the returned results. Note that xx refers to unknown/undefined source or absorber. For IS, QS, MF and temperature parameters, when a single numerical value is given instead of a range, then a ± tolerance range is applied whose absolute value can be given under the "Query Settings" option group depending on the parameter in question

Condition group	Conditions (type)	Example content
Source	Require synchrotron source (selector)	Synchrotron Mossbauer Source
	Require Mossbauer transition (selector)	EU1: Eu-151 (E=21.6 keV)
	Require in source string (list of words)	beamline
	Exclude if source string includes (list of words)	xx Eu2O3
	Require source temperature (positive number or range)	4.2–10
Absorber	Require in absorber string (list of words)	multilayers EuO
	Exclude if absorber string includes (list of words)	xx
	Require number of elements (integer or range)	2–3
	Require elements (list of element symbols)	Eu Nb
	Exclude elements (list of element symbols)	Ir O
	Require absorber temperature (positive number or range)	70–90
Data	Require standard isomer shift (number or range)	−0.5 - 0.1
	Require IS value (number or range)	−0.5 - -0.1
	Require QS value (number or range)	2–3
	Require MF value (number or range)	33
	Require in comments (list of words)	phase transition
	Exclude if comments include (list of words)	magnetic
Authors	Require authors (list of author family names)	list of author family names
	Exclude authors (list of author family names)	list of author family names
	Require author number (integer or range)	1–2
Article details	Require resource type (selector)	Scientific journal
	Require journal (selector)	*Hyperfine Interact.*
	Require in article title (list of words)	analysis Mars
	Exclude if article title includes (list of words)	list of words
	Require volume (string)	33
	Require issue (string)	1–4
	Require page (integer)	199
	Require year (integer or range)	1987–2003
	Require language (selector)	ENG - ENGLISH
Categories and keywords	Require category (selector)	FRO - FROZEN SOLUTIONS
	Require keyword (selector)	BAC - BACTERIA
	Require further keywords (list of keyword codes)	BIO BRM

One of the advantages of such simple textual queries is that they can be easily saved and stored in text files for future reuse (via copy & paste) by the users themselves. As for the queries defined via the conditions available in the condition groups (Table 1), users have the possibility to save query settings into the database for up to two favorite queries. These can

```
SELECT * FROM refs WHERE ( refs.year = 1984 ) AND ( refs.dataisotopes LIKE BINARY '%EU1%' ) AND refs.refkey IN
( SELECT DISTINCT data.refkey FROM data WHERE ( data.isocode = 'EU1' ) AND ( data.stis >= 2 ) AND ( data.stis
<= 3 ) ) ORDER BY refs.year DESC, refs.refkey ASC LIMIT 0, 100
```

Fig. 4 SQL Select statement translated from the query conditions resulting in the query result shown in Fig. 3

```
SELECT * FROM refs WHERE ( refkey = '71M022' ) AND ( authors LIKE '%Mossbauer%' ) AND ( authors LIKE '%Wagner%'
) AND ( dataisotopes LIKE BINARY '%IR3%' ) AND ( dataisotopes LIKE BINARY '%FE7%' ) AND ( elements LIKE BINARY
'%.Ni.%' ) AND ( keywords LIKE BINARY '%|MAA|%' ) AND ( year >= 1970 ) AND ( year <= 1980 ) AND ( journal LIKE
'%Phys. Chem.%' ) AND (( vol = '26' ) OR ( vol LIKE '26-%' )) AND (( pages = '343' ) OR ( pages LIKE '343-%' ))
AND ( title LIKE '%Nuclear Gamma%' ) ORDER BY year DESC, refkey ASC LIMIT 0, 100
```

Fig. 5 SQL Select statement translated from the query text *71M022 Mossbauer Wagner IR3 FE7 Ni MAA 1970–1980 "Phys. Chem." v26 p343 "Nuclear Gamma"* entered into the query search box

then later on be reloaded from the database, thereby avoiding the need for the entering of corresponding (possibly) multiple conditions repeatedly.

When publications are compiled into the database, whenever possible corresponding information about the composition of the measured absorber material(s) is retrieved as well, which then becomes entered into the *Absorber* field of the MEDC core database, mostly either in the form of a chemical formula (e.g. "Fe3O4") or as a compound/mineral name (e.g. "magnetite"). This information may be utilized to enable formulation of queries regarding the elemental composition (i.e. the kinds of elements the absorber is composed of) of the measured absorber materials, which option is rather unique among current bibliographic databases. In order to implement this option in the new WAD system, the MEDC DBM software has been complemented with an algorithm that is able to identify the kinds of elements the absorber includes on the basis of the chemical formula given in the *Absorber* field, which information is then placed in another (*Elements*) field of the same record. For absorbers that are defined by a compound/mineral name in the *Absorber* field, the algorithm attempts to substitute the given names with the associated chemical elements first. For this purpose, a list has been compiled of above 400 mineral names and their typical included chemical elements, on the basis of which the algorithm is able to populate the *Elements* field on the basis of mineral names. Besides minerals, the algorithm also recognizes other textual information (e.g. common element and compound names) in the *Absorber* field. Working of the algorithm is illustrated in Table 2, where examples are given for *Absorber* field contents together with the corresponding automatically determined contents of the *Elements* field.

The contents of the *Elements* field are exported to the new WAD system as well, which makes it possible to query records on the basis of the elements included in the absorber materials. In the WAD system, the advantage of having mineral names previously recognized (by the MEDC DBM software) concerning their included elements will be that by searching for records about absorbers made of specific elements one can also receive those records as returned answers where the absorber is given not with a chemical formula, but with a name of the compound/mineral measured. For example, searching for records about absorbers containing the elements Fe and S, one also receives records where the *Absorber* field contains only "pyrite".

Another advantage of having the information on the kind of elements included in the measured absorber material available is that one can also formulate a condition regarding the number of elements included in the absorber materials searched for. For example, searching for records associated with absorbers including the elements Fe and Dy, one finds that there is a large number (550+) of records satisfying this criterion. If, however, one is interested only in binary alloys of Fe and Dy, one can additionally require the number of elements included in the absorber to be exactly two, in which case the corresponding query (currently) returns only 96 reference records, with most of the matching datasets indeed being about binary alloys of Fe and Dy (along with some others dealing with Fe/Dy multilayers and a few mismatches). After the further exclusion of publications not being related to Fe-Dy binary alloys, there

Table 2 Examples of *Absorber* field contents along with the corresponding *Elements* and *Absorber.HTML* field contents determined automatically by the MEDC DBM program, and the way the latter HTML content is rendered in a web browser

Absorber field content	Elements field content (automatically determined)	Absorber.HTML field content (automatically determined)	Absorber.HTML as rendered in a web browser
alpha-Fe2O3	.Fe.O.	α‑Fe\<sub\>2\</sub\>O\<sub\>3\</sub\>	α-Fe$_2$O$_3$
Et3SnN(NO2)Me	.C.H.N.O.Sn.	**Et**$_3$SnN(NO$_2$)Me	**Et**$_3$SnN(NO$_2$)Me
pyrite	.Fe.S.	pyrite	pyrite
iron sorbed montmorillonite	.Al.Ca.Fe.H.Mg.Na.O.Si.	iron sorbed montmorillonite	iron sorbed montmorillonite
Me4Sn on Al silicate	.Al.C.H.O.Si.Sn.	\<b\>Me\</b\>\<sub\>4\</sub\>Sn on Al silicate	**Me**$_4$Sn on Al silicate
(Fex,Al(1-x))NH4(SO4)2-12H2O	.Al.Fe.H.N.O.S.	(Fe\<sub\>1-\<i\>x\</i\>\</sub\>, Al\<sub\>1-\<i\>x\</i\>\</sub\>) NH\<sub\>4\</sub\> (SO\<sub\>4\</sub\>)\<sub\>2\</sub\> ·12H\<sub\>2\</sub\>O	(Fe$_x$,Al$_{1-x}$) NH$_4$(SO$_4$)$_2 \cdot$12H$_2$O

remain 71 relevant references. From these, in their article title only 10 included "alloy", and none of them included "binary", suggesting that a corresponding literature survey based exclusively on the article titles most probably could not produce results with similar accuracy.

On the basis of chemical formulas in the *Absorber* field, the MEDC DBM software also automatically derives the content of the *Absorber.HTML* field that represents a HTML version of the chemical formula formatted for better readability. By applying a few formattings to the original plain text of the *Absorber* field (notably by formatting numbers of atoms in chemical formulas as subscripts), the formulas may appear in the new WAD system in a familiar way that is easier to recognize/read than the simple text version of the same (see Table 2 for examples).

Another unique feature of the MEDC core database is that it includes Mössbauer parameter datasets with explicitly given values of the isomer shift (IS), quadrupole splitting (QS) and (hyperfine or apparent) magnetic field (MF) parameters for a large number of data records dealing with compounds whose Mössbauer spectrum displays a single, well defined component. The number of data records with explicitly given IS, QS or MF values exceeds, respectively, 43,000, 35,000 and 2200 in the current version of the database. In particular, the number of explicitly given ^{57}Fe IS, QS pairs currently exceeds 20,000.

The new WAD system allows one to query database records on the basis of the associated IS, QS and MF values, either by requiring the values to fall in a specific, explicitly given range, or by requiring the values to be equal to a specific value by considering a certain ± tolerance range given separately under the "Query Settings" option group (Fig. 2).

3 Calculation of the standard isomer shift

In the case of IS values the MEDC database stores the values in question given with respect to different isomer shift reference materials, in line with the variability of corresponding practices appearing in different publications. Consequently, as already pointed out previously [8], in order to make queries based on the isomer shift values produce more relevant/complete results, one needs to introduce into the *Data* table of the MEDC core database a new field containing the isomer shift values given with respect to the same isomer shift reference material for all the data records associated with the same Mössbauer transition.

In the current version of the database we have treated this issue for the nuclides / Mössbauer transitions of ^{57}Fe (FE7, 14.4 keV), ^{119}Sn (SN9, 23.8 keV), ^{151}Eu (EU1, 21.6 keV), ^{121}Sb (SB1, 37.2 keV) and ^{197}Au (AU7, 77.4 keV). For these Mössbauer nuclides α-Fe (RT), SnO$_2$ (RT), EuF$_3$ (RT), ^{121m}SnO$_2$ (RT) and Au metal (4.2 K) have been selected as the standard isomer shift reference materials/matrices, respectively, where the assumed temperature of the reference material is given inside parentheses (with RT referring to room temperature). Consequently, in the new WAD system the *standard isomer shift* (see the "Data" condition group in Table 1) is the isomer shift meant with respect to these reference materials in the case of the above listed nuclides. For the rest of the nuclides the standard isomer shift and the IS value (Table 1, the value originally extracted from publications) are currently equivalent.

In order to calculate the standard isomer shift value for a certain data record with the IS value given, on the one hand one needs information on the reference material with respect to which the IS value is meant, on the other hand one needs to know the isomer shift of the reference material in question with respect to the chosen standard isomer shift reference material given above.

As for the isomer shift reference material and the source matrix applied in the measurement, in the *Source* field (meant to hold the corresponding information) of the data records of the MEDC database the following situations may be encountered:

(a) both the source matrix and the IS reference material are given, e.g. in the form of "Rh(IS/Fe)", where Rh refers to the source matrix and IS/Fe means that the given IS value is meant with respect to α-Fe,

(b) the applied source matrix is unknown but the IS reference material is given, e.g. in the form of "xx(IS/SNP)" where "xx" refers to an unknown source matrix,

(c) the applied source matrix is given, but there is no extra information concerning the IS reference material, e.g., in the form of "Pd",

(d) neither the applied source matrix, nor the IS reference material are known, which case is denoted with "xx" written in the *Source* field.

From the point of view of the calculation of the value of the standard isomer shift, cases (a) and (b) above are relatively straightforward given that the IS reference materials are known. For cases (c) and (d), however, one needs to develop a strategy according to which the standard isomer shift becomes calculated from the given IS value.

In the case of ^{57}Fe the IS reference material is explicitly given (via (a) or (b) above) for ca. 72% of the considered records, whereas the same ratio is ca. 29%, 52%, 43% and 40% for the nuclides ^{119}Sn, ^{151}Eu, ^{121}Sb and ^{197}Au, respectively.

As opposed to the accurate calculation of standard isomer shift values meant with respect to a common isomer shift reference material, it is important to emphasize here that with the introduction of the *standard isomer shift* (st.IS) field our aim is to achieve a more complete and correct set of returned records in response to isomer shift related queries, than it was possible before. And this aim can be realized even though due to the lack of information regarding the IS reference material, for some of the records the conversion of isomer shift values (or lack thereof) may fail to produce correct results. The above mentioned strategy needs to be chosen such that it can be expected to result in the lowest probability of miscalculations in practice. On account of the same considerations, in the calculations we also disregard the temperature of the source and that of the IS reference material, as well as disregard small uncertainties possibly existing regarding the knowledge of isomer shifts of various standard materials, which uncertainties are not of significant importance for our present purpose.

The above mentioned strategy needs to provide us with a reasonable guess concerning the IS reference material for all the records for which an IS value is actually given without explicitly given information on the corresponding isomer shift reference material. We base the strategy on the assumption that for a given Mössbauer nuclide the researchers' choice of the IS reference material and their choice regarding the materials to be investigated (and the temperatures applied) are independent from each other. Namely, should this be true, we may expect the $F(x)$ cumulative probability distribution functions ($F(x) = P(\mathrm{IS} \leq x)$ where P denotes probability) of IS values reported with respect to two different IS reference materials to display similar functional dependences shifted relative to each other along the x axis with an amount (roughly) equal to the isomer shift difference between the two IS reference materials in question:

$$F_{\mathrm{IS\ ref}\ (b)}(x) = F_{\mathrm{IS\ ref}\ (a)}(x + (\delta_b - \delta_a)), \tag{1}$$

where δ_a and δ_b denote the isomer shift of the IS reference materials a and b, respectively. For example, we expect

$$F_{Cr}(x) = F_{\alpha Fe}\left(x - 0.147 \text{ mm s}^{-1}\right) \tag{2}$$

to hold approximately, where $F_{\alpha Fe}$ and F_{Cr} refer to the cumulative probability distribution function of IS values reported wrt. α-Fe and Fe in Cr matrix, respectively, and the value -0.147 mm s^{-1} stands for the isomer shift of Fe in Cr matrix wrt. α-Fe. In practice an estimated form of the $F(x)$ cumulative probability distribution functions can be derived on the basis of the relative occurrences of associated IS value data present in the MEDC database. These estimated functions (denoted as $G(x)$ in the followings) have been used to find the most reasonable IS reference materials in cases where these are not explicitly given.

The validity of Eq. (1) is illustrated on Fig. 6 for the case of ^{151}Eu IS data given explicitly either wrt. Eu_2O_3 or wrt. EuF_3 in the MEDC database [13]. Besides the isomer shift ranges associated with Eu^{3+} (around $x \approx 0$ mm s^{-1}) and Eu^{2+} (below about -11 mm s^{-1}) being clearly recognizable, the shift of the two $G(x)$ curves relative to each other can clearly be observed as well, consistently with Eq. (1).

By examining similar curves drawn for the cases where the IS reference material is not explicitly given (Fig. 7), but the applied source matrix is either given to be Sm_2O_3 or SmF_3, in comparison with Fig. 6 it is immediately apparent that the corresponding ^{151}Eu isomer shift values are most likely meant with respect to ^{151}Eu in the source matrix indicated, i.e. the IS reference material may be taken to be identical with the source matrix.

The case when neither the IS reference material nor the source matrix is explicitly given (curve xx in Fig. 7) is controversial, but overall it seems to be a better match for the curve associated with the source matrix SmF_3.
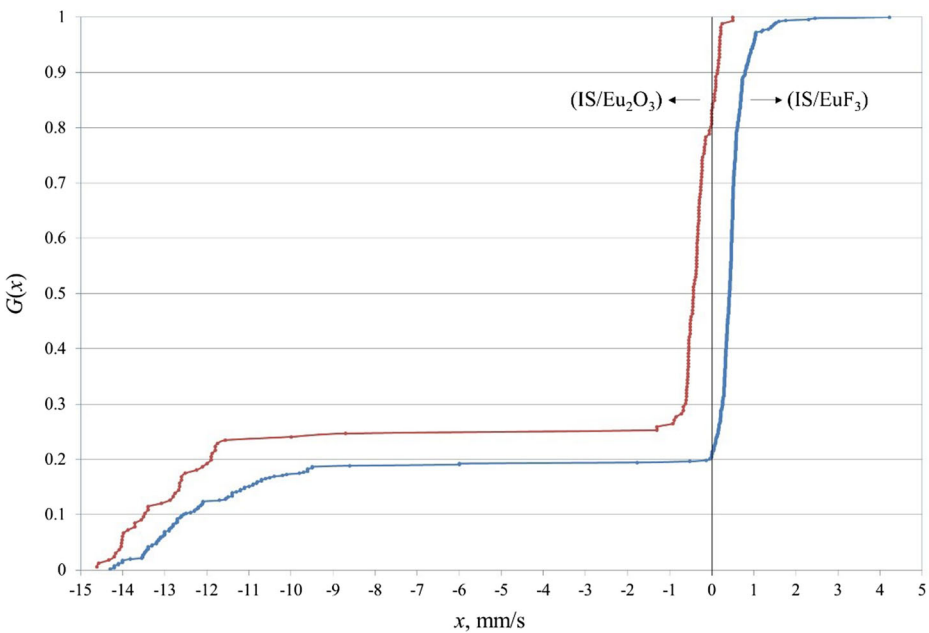

Fig. 6 Illustration of the approximate validity of Eq. (1) for the case of ^{151}Eu IS data where the IS reference material is explicitly given to be either Eu_2O_3 or EuF_3 in the MEDC database [13]. Note that the isomer shift of Eu_2O_3 wrt. EuF_3 is ca. 1.04 mm s^{-1} (Table 3). The relevant parts of the $G(x)$ approximated cumulative probability distribution functions are those where $G(x)$ increases sharply (here around $x \approx 0$ mm s^{-1} and $x \approx -14 \ldots -12$ mm s^{-1}), given that these are the ranges where majority of the IS data occur
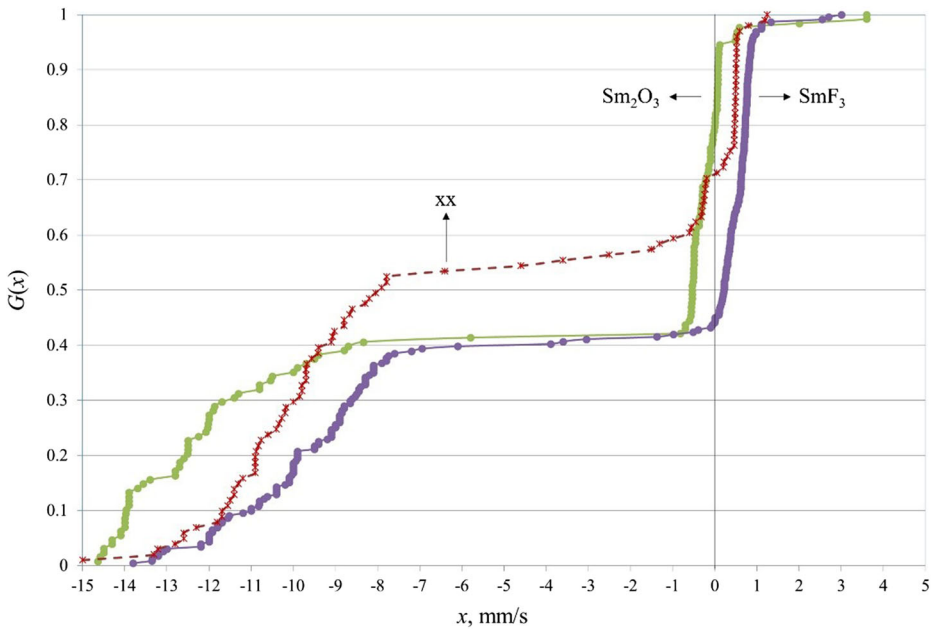
Fig. 7 $G(x)$ approximated cumulative probability distribution functions calculated for [151]Eu IS data where the IS reference material is not explicitly given, and the source matrix is given to be either Sm_2O_3 or SmF_3, along with the case (denoted with xx and dashed line) associated with IS values for which neither the isomer shift reference material nor the source matrix is given in the MEDC database [13]

Based on these observations, the strategy of calculation of the [151]Eu standard isomer shift in cases when the IS reference material is not explicitly given can be as follows.

When the source matrix is given, we assume that the IS value is given with respect to the source matrix, but when it is not given (case xx) we assume that the IS value is given with respect to EuF_3.

The resulting effect of this strategy can be checked in the currend WAD system straightforwardly: when looking for references dealing with Eu-oxides (by requiring elements Eu and O being present in the absorber, and setting the required number of elements to 2) having a [151]Eu IS value in the range of 0.9–1.2 mm s^{-1} we obtain 11 correct references as answer, all referring to Eu_2O_3. When, however, we look for references dealing with Eu-oxides having a [151]Eu standard isomer shift in the range of 0.9–1.2 mm s^{-1} we obtain 19 correct reference matches, all referring to Eu_2O_3.

We note that by assuming EuF_3 as the IS reference material for data records contributing to case xx in Fig. 7, in effect we accept the corresponding IS values as the true standard isomer shift without further conversion. In other cases, where conversion was necessary to obtain the standard isomer shift from the given IS value, the conversion in question was based on the isomer shift values given in Table 3.

Similar analysis of isomer shift values may be performed for the rest of the treated nuclides. For the case of [57]Fe examples are given in Fig. 8 and Fig. 9. Though the curves are not without controversial parts, overall they support the same conclusion as in the case of [151]Eu: whenever the source matrix is explicitly given without the IS reference material, the most reasonable assumption is that the latter is identical with the source matrix. The corresponding conversion

Table 3 Constants used for the calculation of the ^{151}Eu standard isomer shift from the ^{151}Eu IS values given in the MEDC database wrt. various isomer shift standards

If the ^{151}Eu IS value could be assumed to be given wrt. this standard,	then in order to obtain the standard isomer shift value meant wrt. EuF$_3$ at RT, this mm s^{-1} value was added to the IS value.
Eu$_2$O$_3$, Sm$_2$O$_3$	+1.04
EuF$_3$-2H$_2$O	+0.052
EuF$_3$, SmF$_3$	0.0
EuS	−11.54

constants applied for the calculation of the ^{57}Fe standard isomer shift from the IS value given in the database are listed in Table 4 for various source matrices and standard absorbers encountered.

As shown in Fig. 9, the $G(x)$ curve denoted with xx (contributed to by ^{57}Fe isomer shift values where neither the source matrix nor the IS reference material is given) runs rather close to the $G(x)$ curve associated with data records where the IS reference material is explicitly given to be α-Fe (IS/Fe), on which basis it is reasonable to assume that if neither the source matrix nor the IS reference material is known for a ^{57}Fe data record, then the IS reference material can be taken to be α-Fe.

Analogous conclusions could be drawn for the Mössbauer nuclides ^{119}Sn and ^{121}Sb, with corresponding conversion constants being listed in Table 5 and Table 6, respectively. When neither the source matrix nor the IS reference material was known (case xx), then the IS reference material was assumed to be SnO$_2$ (RT) and ^{121m}SnO$_2$ (RT) for ^{119}Sn and ^{121}Sb, respectively.
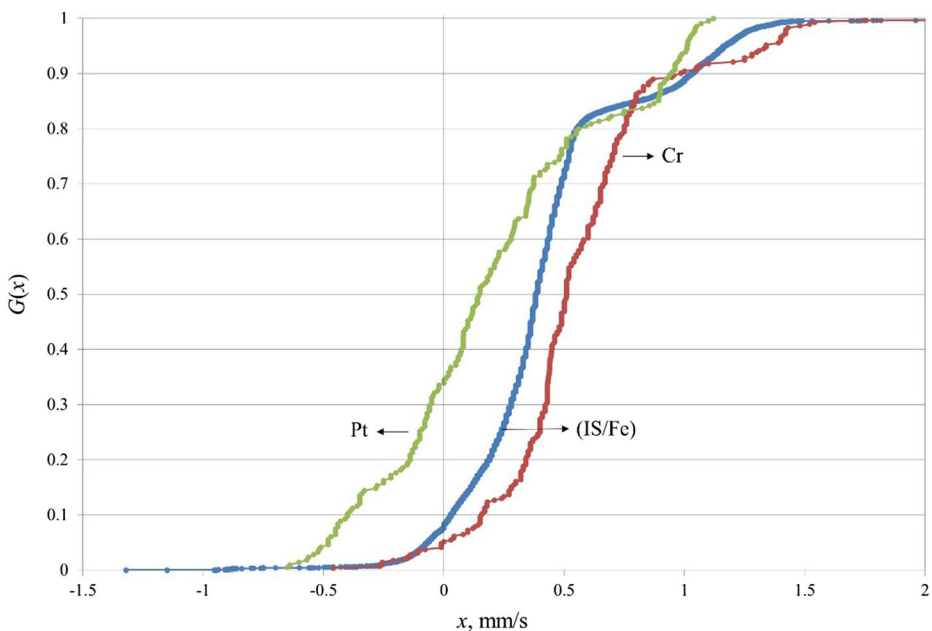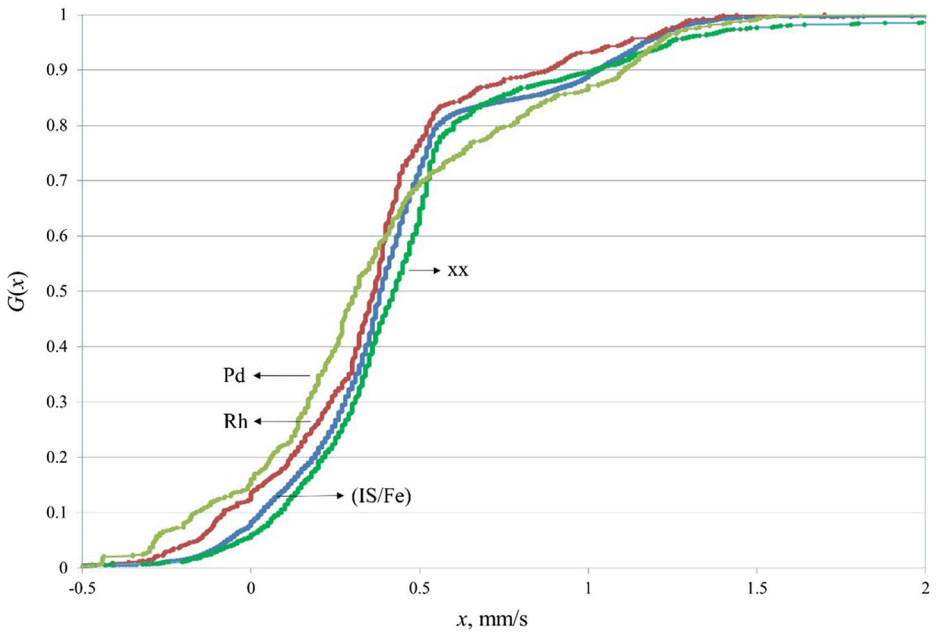

Fig. 8 $G(x)$ approximated cumulative probability distribution functions calculated for ^{57}Fe IS data where the IS reference material is not explicitly given, and the source matrix is given to be either Pt (δ_{Pt} = 0.344 mm s^{-1} wrt. α-Fe) or Cr (δ_{Cr} = −0.147 mm s^{-1} wrt. α-Fe), along with the case (IS/Fe) associated with ^{57}Fe IS values for which the IS reference material was explicitly given to be α-Fe in the MEDC database [13]

Fig. 9 $G(x)$ approximated cumulative probability distribution functions calculated for ^{57}Fe IS data where the IS reference material is not explicitly given, and the source matrix is given to be either Pd ($\delta_{Pd} = 0.170$ mm s^{-1} wrt. α-Fe) or Rh ($\delta_{Rh} = 0.109$ mm s^{-1} wrt. α-Fe), along with the case (IS/Fe) associated with ^{57}Fe IS values for which the IS reference material was explicitly given to be α-Fe in the MEDC database [13]. The curve denoted with xx refers to IS values where neither the IS reference material nor the source matrix was given explicitly

In the case of ^{197}Au the comparison of $G(x)$ curves indicated that whenever an IS value was given without the IS reference material being given explicitly, the latter could be assumed to be

Table 4 Constants used for the calculation of the ^{57}Fe standard isomer shift from the ^{57}Fe IS values given in the MEDC database wrt. various isomer shift standards

If the ^{57}Fe IS value could be assumed to be given wrt. this standard,	then in order to obtain the standard isomer shift value meant wrt. α-Fe at RT, this mm s^{-1} value was added to the IS value.
$KFeF_3$	+1.3
Au	+0.641
Ag	+0.499
alpha-Fe_2O_3 (hematite)	+0.37
Pt	+0.344
Cu	+0.227
Ir	+0.215
Pd	+0.170
Rh	+0.109
Mo	+0.047
Nb	+0.001
Fe	0.0
PFC ($K_4Fe(CN)_6 \cdot 3H_2O$)	−0.047
SFC ($Na_4Fe(CN)_6 \cdot 10H_2O$)	−0.08
SS (all but 310 SS)	−0.09
310 SS	−0.096
Cr	−0.147
SNP ($Na_2Fe(CN)_5NO \cdot 2H_2O$)	−0.257

Table 5 Constants used for the calculation of the [119]Sn standard isomer shift (meant wrt. SnO_2 at RT) from the [119]Sn IS values given in the MEDC database wrt. various isomer shift standards

If the [119]Sn IS value could be assumed to be given wrt. this standard,	then in order to obtain the standard isomer shift value meant wrt. SnO_2 at RT, this mm s^{-1} value was added to the IS value.
SnTe	+3.43
beta-Sn	+2.56
alpha-Sn	+2.03
Mg_2Sn	+1.85
Pd_3Sn	+1.50
SnO_2/$BaSnO_3$/$CaSnO_3$	0.0

Au in Pt matrix. In such cases, in order to obtain the standard isomer shift meant wrt. Au metal at 4.2 K, 1.21 mm s^{-1} was added to the corresponding IS value given in the MEDC database.

The results of the calculations of the standard isomer shift values for the different Mössbauer nuclides were placed in a separate field of the *Data* table of the MEDC database, the original IS values being remained unaltered. Thus, if a more accurate strategy is found for the estimation of the standard isomer shift values on the basis of the original IS values, new calculations may be carried out.

4 Conclusions

A new web accessible online database system (WAD) has been developed in order to facilitate efficient worldwide access to compiled bibliographic and Mössbauer data of the MEDC Mössbauer spectroscopy database via the Internet. The new system achieves progress in this field by making use of the results of recent further developments of the MEDC core database and the associated MEDC DBM database manager software.

The new WAD integrates reference and data queries, and allows users to search the database by considering multiple query criteria concerning Mössbauer parameter data and bibliographical data simultaneously. It is also able to present the returned bibliographical data in conjunction with the associated Mössbauer measurement data records retrieved. It offers a wide range of different query criteria ensuring that users can formulate queries accurately in accordance with their needs.

Automatic interpretation of the *Absorber* field of the MEDC core database (carried out as preprocessing via the MEDC DBM software) allows the new WAD system to execute queries based on the kind of elements included in the measured absorber materials, which option is able to facilitate highly efficient literature surveys in the field of Mössbauer spectroscopy. Automatic formatting of chemical formulas appering in the *Absorber* field (carried out in the

Table 6 Constants used for the calculation of the [121]Sb standard isomer shift (meant wrt. [121m]SnO_2 at RT) from the [121]Sb IS values given in the MEDC database wrt. the given isomer shift standards

If the [121]Sb IS value could be assumed to be given wrt. this standard,	then in order to obtain the standard isomer shift value meant wrt. [121m]SnO_2 at RT, this mm s^{-1} value was added to the IS value.
Ca[121m]SnO_3 / Ba[121m]SnO_3 / [121m]SnO_2	0.0
InSb	−8.7

preprocessing phase) leads to the familiar visualization of chemical formulas that are easier to read and interpret on the screen than the simple textual (unformatted) version of the same formulas.

In the new system an interactivity channel is realized by allowing users to attach comments to records about publications they are coauthor of. Editors and other users who are also coauthors of the same work can read the comments and can add their own, thereby facilitating user feedback and corrections of the record in question, for example.

Overall, the new WAD system offers a highly efficient use of the MEDC database to carry out literature and data searches in the field of Mössbauer spectroscopy.

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