Data Exchange Formats

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Explanatory Notes: With the increasing number of Electrochemical Impedance Applications, the problem of unified data exchange formats becomes important. In addition, the existing computerized experimental facilities produce automatically large sets of data files, which have to be stored, sorted, archived and possibly exchanged via Internet. The efficiency of the data banking and the speed of the virtual research depend notably on the selected Data Exchange Formats (DEF).

The material below describes the DEF for impedance measurements proposed by Zdravko Stoynov [1]. It will be nice if the equipment producers discuss this topic with the end users of their equipment and introduce common data banking as a convenient and appropriate tool, especially for friendly scientific communication in the big EU Framework programs projects.

We offer Zdravko Stoynov's approach since we use it for more than 15 years and find it extremely convenient. Our group is ready to develop and upload free of charge Data Convertor. We shall be thankful for every remark, correction, recommendation or suggestion.

The DEF description which we have included in this special issue of Bulgarian Chemical Communications can be also downloaded from the web site of the European Internet Centre for Impedance Spectroscopy www.accessimpedance.eu (in the Section Information Kit/News).

The web site of EICIS will be upgraded in September/October 2018 with its new name "Zdravko Stoynov Internet Centre for Impedance Spectroscopy

New ideas and approaches are welcome.

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INTRODUCTION

In accordance with the general IUPAC recommendations, the Electrochemical Impedance Spectroscopy's Data Exchange Formats (DEF) should be generic, economic and efficient. Following the practical experience, some other recommendations are useful: DEF should be self-explaining and easily readable by the user as well as by the computers. They should contain enough explanations and to a certain extent should be over-dimensioned by verbal information. The used symbols must be readable by computers of different versions and generations and should be selected only from the ASCII table.

For these reasons, the use of "text only" (xxxxx.txt) format is recommended for the storing and attachment format. The ".txt" format is not only universal, but it is also the most economic. The experimental comparison with ".rtf", ".doc" and other word processing formats shows an excessive enlargement of the file volumes, when stored in those formats. The inefficient enlargement for ".rtf" is about 5 times and for ".doc" extension – about 20 times. For a single file the enlargement can be neglected, but for a data bank, containing thousands of files, and for their exchange, the compactness becomes important.

The ".txt" files have the advantage to be readable by computers of all versions, independent of the type and version of its software and Internet instruments.

Another problem arises when a series of experiments are carried out with one and the same object with a varying parameter. One solution for the DEF efficiency is the application of the Large Structured Files (LSF), proven in our practice.

The LSF starts with a header. The header should contain all the information necessary for the understanding, sorting, exchange and banking of the data.

The LSF contains a certain number of pages. Each page starts with a symbol (#) and a number (1 to *N*) and has a verbal informative label, corresponding to the value of the varying

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parameter. The label contains determination of the size (*n* x *m*) of the data matrix as well as the description of the type of the data (f, Z', Z'', t^o, or others).

After the label comes the data kernel. It contains a number of lines (*n*). Every value in the line is separated from the previous one by ";".

Every page finishes with a tag (@), which could be followed by the post–experimental observations.

The LSF finishes with a footer symbolizing the end of the file (@ EOF).

EXAMPLES

Examples for explanation of the DEF (Large Structured Files) with a code
#ftp:EISDEF205LSF.txt.

The file, stored as xxxxx.txt with this CONVENTION CODE is a Large Structured File (LSF).

The suggested EIS DEFs are illustrated in the following examples:

Large Structure File – Example LSF1:

File Name: BATI043.txt
#ftp:EISDEF205LSF.txt   #fnm:BATI043.txt   pages: 6
<BaTi sample N.33 measured>
<No: 1243-49 author: X. Broun 29-01-2005   20:36:05>
<object: BaTi; sin.crystal [100] S=1.22 cm^2 d=0.2 cm>
<set-up: Sol 1256 + Pot. self-made; cell: planar>
<Udc=0; Uac=5 mV; down; variation: temper. 'C>
#p1   {f; Z`; Z``} [SI] (3*56)
<calibration short connected>
1000;1.356E-3;2.265E-3
…;   …;   …
…;   …;   …
…;   …;   …
0.001;1.222E-3;-0.005E-3
@p   <room temperature>
#p2   {f; Z`; Z``} [SI] (3*56)
<calibr. open>
…;   …;   …
@p
#p3   {f; Z`; Z``} [SI] (3*56)
<object row data   var: 20'C>
…;   …;   …
@p
#p4   {f; Z`; Z``} [SI] (3*56)
<object row   var:31'C>
…;   …;   …
@p
#p5   {f; Z`; Z``} [SI] (3*56)
<object row var: 40'C>
…;   …;   …
@p
#p6   {f; Z`; Z``} [SI] (3*56)
<object row var:51'C>
…;   …;   …
@p
@ EOF

Explanations:

File Name: BATI043.txt

#ftp:EISDEF205LSF.txt   #fnm:BATI043.txt   pages: 6
<BaTi sample N.33   measured>
<No: 1243-49 author: X. Broun   29-01-2005 20:36:05>
<object: BaTi; sin.crystal [100] S=1.22 cm^2 d=0.2 cm>
<set-up: Sol 1256 + Pot. self-made cell: planar >
<Udc=0; Uac=5 mV; down; variation: temper. 'C>
(this information forms the file's header)
#p1 {f; Z`; Z``} [SI] (3*56)   = *page 1 beginner &*
                                             descriptor

<calibration short connected>   = *free text*
1000;1.356E-3;2.265E-3   = *data /example/*
…;   …;   …
…;   …;   …
…;   …;   …
0.001;1.222E-3;-0.005E-3   = *last data*
@p <room temperature>   = *page footer & tag*

 #p2 {f; Z`; Z``} [SI] (3*56)   = *page 2 beginner &*
                                             descriptor

<calibr. open>
…;   …;   …
@p
#p3 {f; Z`; Z``} [SI] (3*56)   = *page 3 beginner*
                                             & descriptor

<object row data. var: 20'C>
…;   …;   …
@p
#p4 {f; Z`; Z``} [SI] (3*56)   = *page 4 beginner &*
                                             descriptor

<object row   var:31'C>
…;   …;   …
@p
#p6 {f; Z`; Z``} [SI] (3*56)   = *page 6 beginner &*
                                             descriptor

<object row   var:51'C>
…;   …;   …
@p   = *last page footer*
@ EOF   = *file footer*

Large Structure File – Example LSF2:

File Name: BATI044.txt
#ftp:EISDEF205LSF.txt #fnm:BATI044.txt pages: 8
<BaTi recalculated from BATI043.txt corrected Z & Y >
<No: 1250-58 author: X.Balan   30-01-2005
21:36:05>
<object: BaTi; sin.crystal [100] S=1.22 cm2 d=0.2 cm>
<set-up: Sol 1256 + Pot. self-made cell:planar>
<Udc=0; Uac=5 mV; down; variation: temper. `C>
#p1   {f; Z`; Z``} [SI] (3*26)
<calibration short connection>
…;   …;   …
@p
#p2   {f; Z`; Z``} [SI] (3*56)
<calibr. open>
…;   …;   …
@p
#p3   {f; Z`; Z``} [SI] (3*56)
<object row data.   var: 20`C>

…;   …;   …
@p
#p4   {f; Z`; Z``} [SI] (3*56)
<object data corrected LCcell   var:20`C>
…;   …;   …
@p
#p5   {f; Y`; Y``} [SI] (3*56)
<object corrected;   Y   var:20`C>
…;   …;   …
@p
#p6   {f; lg |Y|; phi} [SI] (3*56)
<object corrected;   Bode   var:20`C>
…;   …;   …
@p
#p7   {f; Z`; Z``} [SI] (3*56)
<simulated M11= La: R C/R BW >
<par: 120; 1.23E-3; 1038; 30246\880 >
<identified by CNLS – Boukamp version "3/2000" for 20'C>
…;   …;   …
@p
#p8   {f; Z`; Z``} [SI] (3*56)
<residuals f; dZ`/Z`; dZ``/Z``>
…;   …;   …
@p
@ EOF

Remarks:

1. The symbol "#ftp:EISDEF205LSF.txt" describes the file's type in accordance to this convention.

2. The symbols "(", ")", "\" and "var:" are for computer reading. They possess the dimensions of the data kernel matrix and the varying parameter's values.

3. The text within the symbols "<" and ">" is for the user's reading; its internal format is free.

4. The number of the text lines <………> is unlimited.

5. The value of the varying parameter should immediately follow the symbol "var:" ("var:" is for computer reading!).

6. The symbols "{","}", "[","]", "#ftp:" and "#fnm:" are for computer reading.

7. The data kernel may contain additional data for every frequency: time of measurement, quality of measurement, d.c. values and others.

8. The page footer is optional.

9. The file footer is optional.

Explanations:

#ftp:	= ***computer used symbol***
EISDEF205LSF.txt	= ***file type***
#fnm:	= ***computer used symbol***
BATI033.txt	= ***file name given by the operator***
<BaTi sample N.3 measured>	= ***text:object***
<No:1232 author: X.Green 29-01-2005 20:36:05>	= ***text:number***
<object: BaTi; single crystal[100] S=1.22cm2 d=0.2cm>	= ***object***
<set-up: Sol 1256 + Pot. self-made cell:planar>	= ***set-up***
<Udc=0; Uac=5 mV; down; temper. 22`C>	= ***meas.cond.***
# {f; Z`; Z``} [SI] (3*26)	= ***data descriptor***
…; …; …	= ***data***
…; …; …	= ***last data***
@p	= ***page footer = end page***

Additional Explanations:

file name:	- ***name of the file given by the author;***
file type:	- ***STANDARD, subject to this preliminary convention;***
<text>:	- ***free text, composed by the author, including information about the author, date/time, object, instrumentation, measurement conditions; other information.***
<text>	- ***a number of lines with <… …> is free.***
# {f; Z`; Z``} [SI] (3*26)	- ***descriptor of the following data:***
#	- ***computer used symbol (new page)***
{f; Z`; Z``}	- ***descriptor of data types***
[SI]	- ***descriptor of data units /in this case in SI/***
(3*26)	- ***data kernel format***
( )	- ***computer used symbol***
\	- ***computer used symbol***
3*26	- ***in this example: 3 columns, 26 lines***
# { } [ ] \: \ < > #ftp #fnm @p	- ***computer used symbols***

Additional Explanations of the file type descriptor:

#ftp:EISDEF205LSF.txt	- ***file type code***
#ftp:	- ***computer used record of file type***
EIS	- ***Electrochemical Impedance Spectroscopy***
DEF	- ***Data Exchange Format***
205LSF	- ***2005 year, Convention LSFile***
.txt	- ***<u>type in which the file must be saved / attached</u>***

REFERENCES

1. Z. Stoynov, D. Vladikova, Differential Impedance Analysis, Marin Drinov Academic Publishing House, 2005, pp, 207-213.

Формати за обмен на данни

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Обяснителни бележки: С нарастване приложенията на електрохимичната импедансна спектроскопия, проблемът с унифициране на форматите за обмен на данни става все по-съществен. Успоредно с това съществуващите компютризирани измервателни системи автоматично генерират огромен брой файлове с данни, които трябва да бъдат съхранявани, сортирани, архивирани и обменяни чрез интернет. Ефективното съхранение на данни и разрастването на виртуалната колаборация зависят силно от избраните формати за обмен на данни (ФОД).

Предлаганият материал описва ФОД за импедансни измервания, предложени от Здравко Стойнов [1]. Би било полезно, ако производителите на оборудване дискутират тази тема с крайните си потребители и въведат общоприета форма за съхранение и обмен на данни като удобен и подходящ инструмент, особено полезен за научна комуникация в големи проекти по рамковите програми на ЕС.

Ние предлагаме подходът на Здравко Стойнов, който използваме повече от 15 години и който намираме за изключително удобен. Нашата група е готова да разработи и да качи безплатно *Конвертор на данни*. Ще бъдем благодарни за всяка забележка, корекция, препоръка или предложение.

Описанието на ФОД което включваме в това специално издание на Bulgarian Chemical Communications, може да бъде изтеглено и от уеб сайта на Европейския интернет център по импедансна спектроскопия (EICIS): www.accessimpedance.eu (в секция Информация / Новини).

Уеб сайтът на EICIS ще бъде актуализиран скоро с новото си име "Интернет център за импедансна спектроскопия „Здравко Стойнов".

Ще се радваме на нови идеи и подходи.

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