Instructions for using BL14B2 XAFS Standard Sample database (Ver. BENTEN)

11.24.2022 Hironori Ofuchi

- 1. Connecting to a database site
- (1) Open the SPring-8 experimental data transfer system BENTEN (URL: <u>https://benten.spring8.or.jp/</u>). When you open the URL, the top page (Fig. 1) is displayed.

SPring 8 Experimental Data Transfer System	
Login Username:	
Guest login with Email if you only need open data access.	
BENTEN SYSTEM:Copyright (C) 2020 JASRI All Rights Reserved.	 利用に関してはSPring-8 BENTENデータペースユーザーマニュアルを参照ください。 BENTEN SYSTEMではCookieを利用しています。 Cookieの使用目的は利用者のログイン認証と CSRF対策、ウェブサイトの利便性用途のみ に限定しております。

 Please refer SPring-8 BENTEN database User Manual (Japanse only for now).
 BENTEN SYSTEM uses cookies. The purpose of using cookies is limited only to user authentication, CSRF protection, and convenience of website.



(2) UI site (SPring-8 / SACLA electronic application system (https://user.spring8.or.jp/)), Enter your user name (SPring-8 ID) and password, and click the Login button. To log in with your personal email address, click "Guest login with Email" under the Login button. The guest login screen shown in Figure 2 will be displayed. Enter your email address and click the Login button. If you log in normally, the screen (Fig. 3) related to email address authentication (two-factor authentication) will be displayed.

*After creating a new UI site account, it will take about a day to log in to this database site.

SPringe 8 Experimental Data Transfer System	
Guest Login Email:	
BENTEN SYSTEM:Copyright (C) 2020 JASRI All Rights Reserved.	 利用に関してはSPring-8 BENTENデータベースユーザーマニュアルを参照ください。 BENTEN SYSTEMではCookieを利用しています。 Cookieの使用目的は利用者のログイン認証とCSRF対策、ウェブサイトの利便性用途のみに限定しております。
	 Please refer SPring-8 BENTEN database User Manual (Japanse only for now). BENTEN SYSTEM uses cookies. The purpose of using cookies is limited only to user authentication, CSRF protection, and convenience of website.





Fig. 3

(3) Click "Send Email" button. Following screen is displayed (Fig. 4).



Fig. 4

(4) Check e-mail of subject "Guide for BENTEN authentication" in your e-mail software (Fig. 5)
 Guide for BENTEN authentication

実験データ転送システムBENTENの認証を行う際は以下URLをクリックしてください。

https://benten.spring8.or.jp/verify/token/confirm

有効期限: 20分

このメールに見覚えがない場合はメールを破棄していただいて結構です。

To proceed the email authentication process of BENTEN, please click the URL below.

https://benten.spring8.or.jp/verify/token/confirm

Expiration time : 20 min.

Please ignore this message if you did not make the request.

Fig. 5 BENTEN authentication e-mail

(5) When you click the link in the e-mail, a screen will be displayed to prompt for authentication (Fig.6).



Fig.6

(6) Click "Authenticate" button. The authentication completion screen is displayed (Fig. 7)



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Fig. 7 Authentication completion screen

(7) The email sending screen in Fig. 4 is redirected to the data viewing screen (Fig. 8).



Fig. 8 Data viewing screen

2. Browsing standard sample data

2-1. Viewing data

(1) In the tree display on the left side of the screen, the screen shown in Fig. 9 (a) is displayed. The folder hierarchy of the tree is

- root(Fig. 9 (a))
- SPring-8(Fig. 9 (b))
- BL14B2(Fig. 9 (c))
- XAFS_Standard (Registration folder for XAFS standard sample data、 Fig. 9 (d))
- Element(Fig. 9 (e))
- Absorption edge(K,L3,2,1、Fig. 9 (f))
- Net plane(Si(111) or Si(311), Fig. 9 (g))
- Name of standard sample(Fig. 9 (h))

It is in the order of. In the corresponding data field, the information of the folder one level below the folder selected in the tree display (in the case of the lowest layer, the data file included in the folder) is displayed.

SPring 8 Experimental Data Transfer System		UID:	LOGOUT
Search under folder your pr	TOPOSAI V DOWNLOAD CHECKED ITEMS		
Select root SPring-8 Tree display	CDL FILE NAME		
	Corresponding data		
	\$		
	Corresponding data		
	thumbnail image		
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BENTEN SYSTEM:Copyright (C) 2019 JASRI All Rights Reserved.			

Fig.9 (a) Initial screen for tree display (select the top (root) of the tree display)

SPring 8 Experimental Data Transfer System		LOGOUT
Search under folder your proposal 🗸 🕻	DOWNLOAD CHECKED ITEMS	
Select SPring-8 BL14B2	S DDL FILE NAME D DL BL1482	^
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	KEY VALUE	
<	<	>
BENTEN SYSTEM:Copyright (C) 2019 JASRI All Rights Reserved.		

(b) Selecting SPring-8 folder

SPring• 8 Experimental Data Transfer System		LOGOUT
Search under folder your proposal V DOWNLOAD CHECKED ITEMS		
Image: Spring-S Select BL14B2 Image: Spring-S Select BL14B2	C PILE NAME	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
Z Z Z Z Z Z Z Z Z Z Z Z Z Z	c	~

(c) Selecting BL14B2folder







(e) Selecting element folder (ex. Cu folder)



(f) Selecting absorption edge folder (ex. K)



(g) Selecting net plane folder (ex. 111)



(h) Selecting sample name folder (ex. Cu-foil)

2-2. Browsing experimental data information

(1) Select the folder of the sample you want to browse from the tree display and display the corresponding data screen (Fig. 10).

SPring- 8 Experimental Data Transfer System		UID: LOGOUT
	Search under folder your proposal V	
Image: Second		× ×

Fig.10 Display of applicable data screen (selecting Cu-foil folder)

(2) Click any of the data in the corresponding data screen on the upper right. Click to display experimental data information (Fig. 11 (a) thumbnail image, (b) simple information).





(b)

Fig.11 Experiment data information screen

(a) Thumbnail image (b) Simple information(Scroll down the lower right screen)

2-3. Types of experimental data

(1) In the BL14B2 XAFS standard sample database, 3 types of experimental data (extensions dat, ex3, txt ((5 types if fitted encoder processing is available)) for one registration number, and detailed information of the experimental data. (metadata.main.yml, metadata.data format.yml, metadata.data info.yml) is registered.

	FILE NAME
	Pd-K_Pd-foil_Si111_50ms_150511.dat
FILE NAME	Pd-K_Pd-foil_Si111_50ms_150511.ex3
Cu-K_Cu-foil_Si111_50ms_120613.dat	Pd-K_Pd-foil_Si111_50ms_150511.bt
Cu-K_Cu-foil_Si111_50ms_120613.ex3	Pd-K_Pd-foil_Si111_50ms_150511_fe.ex3
Cu-K_Cu-foil_Si111_50ms_120613.bd	Pd-K_Pd-foil_Si111_50ms_150511_fe.bd
Cu-foil.thumb.png	Pd-foil.thumb.png
metadata.data_format.yml	metadata.data_format.yml
metadata.data_info.yml	metadata.data_info.yml
metadata.main.yml	metadata.main.yml
(a)	(b)

Figure 12 Database registration data ((a) Cu-foil, (b) Pd-foil)

The measurement information is described in the file name of the experimental data in the following order.

Element-Absorption edge-Sample name-Net plane-Dwell time-Measurement date-(fe).Extension

An example of the measurement information shown in the file name of each registered data in FIG. 12 is shown below.

(Example 1) Cu-K_Cu-foil_Si111_50ms_120613.dat

Element: Cu Absorption edge: K-edge Sample name: Cu-foil Net plane: Si (111) Dwell time: 50msec per point Measurement date: June 13, 2012 Extension: dat (9809 format)

(Example 2) Pd-K_Pd-foil_Si111_50ms_150511_fe.txt Element: Pd Absorption edge: K-edge Sample name: Pd-foil Net plane: Si (111) Dwell time: 50msec per point Measurement date: May 11, 2015 fe: With fitted encoder processing (*) Extension: Readable by XAFS analysis software Athena

((*) Refer to Appendix I about fitted encoder processing)

Table 1 shows the file formats of the experimental data extensions.

Extension	File type
dat	Measurement data (9809 format)
ex3	Readable by XAFS analysis software REX2000
txt	Readable by XAFS analysis software Athena

Table 1 Extension file for	rmat
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The file with the extension yml contains information such as standard samples, measurement conditions, measurement data, and main items. These are YAML-formatted text files that can be viewed with a text editor or browser (Fig. 12). Currently, three types of metadata.main.yml, metadata.data_format.yml, and metadata.data_info.yml are registered. Table 2 shows the items in each yml file.

	sample:
	- chemical_formula: PbO
	lot_number: '5018791'
	model_number: PBO11PB
	name: Lead(II) oxide
	supplier: KOJUNDO CHEMICAL LABORATORY
	tag: main
	- chemical_formula: Pb-foil
	model_number: PB000100
10	name: Lead
11	supplier: Goodfellow
12	tag: reference
13	measurement:
14	method:
15	category: spectroscopy
16	sub_category: XAFS
17	absorption_edge: Pb L3-edge
18	instrument:
19	slit:
20	- name: 4Dslit
21	vertical_size[mm]: 1.0
22	horizontal_size[mm]: 5.0
23	xafs:
24	10:
25	element_number: 1
	element:
27	- type: Ion Chamber
28	gas: N2 75% + Ar 25%
29	HV[V]: 1000.0
	amp_gain[V/A]: 10000000.0
31	I1:
32	element_number: 1
33	element:
34	- type: Ion Chamber
	gas: Ar 100%
36	HV[V]: 1000.0
37	amp_gain[V/A]: 10000000.0
38	12:
39	element_number: 1
40	element:
41	- type: Ion Chamber
42	gas: Ar 100%
43	HV[V]: 1000.0
44	amp_gain[V/A]: 100000000.0
45	local:
46	<pre>measurement_time[sec]: 235.0</pre>
47	<pre>xafs_filename_list:</pre>
48	- Pb-L3_Pb0_Si111_50ms_210209.dat

Fig.12

sample (Category of sample)	
chemical_formula	Chemical formula of the sample
lot_number	Lot number of the sample
model_number	Model number of the sample
name	Substance name of the sample
supplier	Supplier name of sample
tag	The sample (main, measured by I0-I1 detector) or reference sample (reference, measured by I1-I2 detector)
measurement (Category of me	asurement parameters)
category	Measurement method category
sub_category	Measurement method subcategory
absorption_edge	Measuring element and absorption edge
instrument (Category of measuring instrument)	
vertical_size [mm]	4D slit size ((W) width)
horizontal_size [mm]	4D slit size ((H) height)
type	Types of I0, I1 and I2 detectors
gas	Type of gas used for I0, I1 and I2 detectors
HV [V]	Applicable voltage value to I0, I1 and I2 detectors
amp_gain [V / A]	Gain value of I0, I1 and I2 detectors
local	
measurement_time [sec]	Time taken from the start to the end of measurement
xafs_filename_list	File name of experiment data (9809 format)

Table 2 Items listed in the yml file (a) metadata.main.yml

(b) metadata.data forma	at.yml
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xafs_raw_data_format (Category of measurement data)		
extension	extension	
name	item name	
unit	unit	
additional_metadata Additional information for each item		
xafs_processed_data_format (Category of converted data)		

extension	extension
name	item name
unit	unit
formula	Conversion formula from measurement data
additional_metadata	Additional information for each item

(c)	metadata.data	info.vml
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proposal_number	proposal number	
access_rights	Access rights	
data_depositor (Category of data writer)		
name	Name of the data writer	
organization	Data writer's organization	
contact_name (Category of data responsible)		
name	ame Name of the data manager	
organization	Data responsible organization	
role	The role of the data manager	

- 4. Download experimental data
- 4-1 How to download data
- (1) Check the experimental data of the sample you want to download (Fig. 14).



Fig. 14 Experimental data information screen (Cu-foil)

(2) Click the "DOWNLOAD CHECKED ITEMS" button on the screen. A zip file save message will be displayed, so save it in any folder.

SPring. 8 Experimental Data Transfer System		UID
		Search under folder your proposal V
	include related data files DOWNLOA DL FILE NAME Cu-K_Cu-foil_SI111_50ms_120613.d Cu-K_Cu-foil_SI113_50ms_120613.b Cu-K_Cu+foil_SI113_50ms_120613.b Cu-foil thumb png metadata data_it_normatymi metadata_data_it_normatymi metadata_data_it_normatymi metadata_data_it_normatymi	DICHECRED ITEMS
Conner nickel	KEY	VALUE
Cu(CH3COO)2(neutral)	@system@parent_directory	/SPring-8/BL14B2/XAFS_Standard/Cu/K/111
- (NO3)2_3H2O	@system@uuid_register_directory	/storage/volume-01/SPring-8/BL14B2/2020-04/4b31e8e3-1c70-4f30- 974f-8aed46931ecc
	@system@version@agent	1.0.2
🛄 Cu2O	@system@version@data_register	0.5.4
— 🥘 Cu2S	@system@version@metadata	spring8-bl14b2-2020.04.21
	@subject@access_rights	open
	@subject@class_name	BL14B2
CuCO3(basic)	@subject@correspondance	Industrial Application Division
- 🚇 CuCl	@subject@correspondance@affiliation	JASRI
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Fig. 15 Experiment data save screen (for Microsoft Edge)

4-3 How to download multiple data

(1) If you want to download multiple data at once, check the check box of the data you want to download and click the "DOWNLOAD CHECKED ITEMS" button (Fig. 16 (a)-(c)).

SPring 8 Experimental Data Transfer System		UID:	LOGOUT
Search under folder your proposal >> DOWNLOAD CHECKED ITEMS			
	DL FILE NAME C320116Cult8_plan C320116Cult8_plan C320116Cult8_plan C320116Cult8_plan C320116Cult8_plan CC320116Cult8_plan C CC20116Cult8_plan C CC20116Cult8_plan C CC20116Cult8_plan C CC20116Cult8_plan C CC2010Col20plands10_plan C CC20102Dplands10_plan C		× ×

Fig. 16 (a) Downloading for each sample folder



(b)Downloading for each net plane folder

SPring 8 Experimental Data Transfer System		LOGOUT
Search under folder your proposal V DOWNLOAD CHECKED ITEMS		
🚈 🛄 root		^
A- 🦲 SPring-8		
A BL14B2		
A SAFS_Standard		
p- L Ag		
Au		
	Fe	
S- III Er		
Eu		
- 🛺 Fe		
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þ- 🛺 La		
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D = 40 Nb	KEY VALUE	
0- 🛄 Nd		
D- 40 Ni		
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ồ- 🚨 data	× (~
BENTEN SYSTEM Convrint (C) 2019 JASBI All Rights Reserved)

(d) Downloading for each element folder

Appendix

I. Fitted encoder processing for Angle selection

In the beamline BL14B2, short-period vibrational components different from EXAFS vibrations sometimes overlap on the high-energy side of XAFS spectra measured in the high-energy region. As example, the normalized EXAFS of $Pd(NH_3)_4Cl_2 \cdot H_2O$ measured at the Pd-K edge and Si(111) net plane is shown in Fig.17. As the wavenumber increases, the short-period vibrational component becomes more pronounced. This short-period vibrational component is not due to the sample, but to the encoder of the crystal monochromator.



Fig.17 Normalized EXAFS of Pd(NH₃)4Cl₂ · H₂O (Pd-K, Si(111) net plane) (Angle(o) is specified for Angle selection when converting data with XAFS_DataConverter.)

Figure 18 shows the angles of the crystal monochromator (PC and encoder values) when the XAFS spectrum in Fig. 17 was measured, and it can be seen that there is a periodic shift in the encoder values with respect to the PC angle. Since the sample-derived vibrational component is larger at the low wavenumber side of the normalized EXAFS, the effect of this periodic vibration is negligible. However, at the high wavenumber side, where the amplitude of the vibration component becomes smaller, the effect cannot be ignored, and a short periodic vibration component appears as shown in Fig.17. This periodic vibration of encoder values is not a problem specific to the beamline BL14B2, but is also seen in other beamlines. (This has been confirmed at the beamline BL19B2 and BL46XU. However, the degree of periodic deviation and the energy region where the deviation occurs vary from beamline to beamline. In most cases, the periodicity is much different compared to the EXAFS oscillation component, so the measured data are not affected).



(From the file created by "Output Excel file (for angle correction confirmation)" in XAFS_DataConverter)

The XAFS data conversion program corrects for this periodic shift using a polynomial approximation (red line in Fig. 18) by processing the fitted encoder. Figure 19 shows a comparison of the normalized EXAFS spectral shape with and without the fitted encoder process, and it can be seen that the fitted encoder process eliminates the short-period vibration component on the high wavenumber side.



Fig.19 Normalized EXAFS of $Pd(NH_3)_4Cl_2 \cdot H_2O$ (Pd-K edge, Si(111) net plane) (Blue line: without fitted encoder processing, red line: with fitted encoder processing)

When fitted encoder processing is performed, the XANES spectrum is modulated from the original data as shown in Fig.20. Therefore, when discussing XANES spectra, care should be taken not to mix fitted encoder processed data with non-fitted encoder processed data.

In addition, not all encoder-derived vibration components appear on the high wavenumber side of all EXAFS spectra in the high-energy region. Figure 21 shows the normalized EXAFS of $Pd(NH_3)_4Cl_2 \cdot H_2O$ measured on the Si(311) net plane, and unlike the measurement on the Si(111) net plane, no short-period vibration component is observed on the high wavenumber side, and the spectrum shape is almost unchanged after fitted encoder processing. Therefore, it is possible to determine whether the short-period vibration on the high wavenumber side originates from the encoder or not by comparing the spectrum without fitted encoder processing (Angle(o)) and with fitted encoder).



Fig.20 XANES spectra of $Pd(NH_3)_4Cl_2 \cdot H_2O$ (Pd-K edge, Si(111) net plane) (Blue line: without fitted encoder processing, red line: with fitted encoder processing)



Fig.21 XANES spectra of $Pd(NH_3)_4Cl_2 \cdot H_2O$ (Pd-K edge, Si(311) net plane) (Blue line: without fitted encoder processing, red line: with fitted encoder processing)

Revision history

Revision date	Reviser
3.31.2022	Hironori Ofuchi
11.24.2022	Hironori Ofuchi