



International Atomic Energy Agency

Technical Remarks on Compilation

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New Verification of EXFOR Data by Koning

Data Bank
NEA/DB/DOC(2014)3
www.oecd-nea.org

Statistical Verification
and Validation of the EXFOR
database: (n,n'), (n,2n), (n,p),
(n, α) and other neutron-induced
threshold reaction cross-sections

Now available!
<http://www.oecd-nea.org/databank/docs/2014/db-doc2014-3.pdf>

 **OECD**
BETTER POLICIES FOR BETTER LIVES

 **NEA**
NUCLEAR ENERGY AGENCY

Arjan Koning evaluated a deviation factor (Michel's f-factor) for neutron-induced threshold reaction cross sections in EXFOR from those in various libraries (CENDL-3.1, EAF-2010, ENDF/B-VII.1, IRDFF-1.0, JEFF-3.2, JENDL-4.0, TENDL-2013 as well as TALYS calculation when necessary).



New Verification of EXFOR Data by Koning (cont)

Work done by Arjan (from the report)

“All (n,n') , $(n,2n)$, (n,p) , (n,α) cross sections, plus other less measured (n,x) cross sections like (n,d) , (n,t) , (n,h) , (n,np) and $(n,n\alpha)$ etc, i.e. about **10000 subentries** out of a total of about 25000, have been covered in more detail than just automatic comparison.”

“Put differently, the only reaction classes *not reviewed* are (n,tot) , (n,el) , (n,non) , (n,f) and (n,γ) . “



New Verification of EXFOR Data by Koning (cont)

Important conclusions for us (from the report)

“In most cases, it turned out that the reported quantity was indeed correctly compiled into EXFOR.”

“However, for about 30 cases, the EXFOR compilation was wrong, for either the numerical value or the reported quantity, and appropriate actions have in the mean time been taken by NRDC to correct this.”

“More important than these errors is the confirmation that many experiments for the various reactions have indeed been correctly compiled.”



New Verification of EXFOR Data by Koning (cont)

Important conclusions for us (from the report)

It is recommended that at least the status symbol of each data set, i.e. T, R, N or E, is recorded in EXFOR or a related database.

T: Subentries which are automatically compared with data libraries

R: The subentry contains certainly the reaction and data measured by the author, since the associated publication has been checked by the reviewer.

N: Automatic score T1, T2 or T3 but pdf of paper not available for checking.

E: Subentries which contain errors and require specified action

(For each symbol, 1: small deviations. / 2: questionable deviations /3: strong deviations, e.g., T1, T2, T3, R1, R2, R3,...)

The final score must be T1, N1, N2, N3, R1, R2 or R3 for verified subentries. **Keep R (checked against the article) in the EXFOR Master?** (~3000 data sets)



Digitization – Comment on X4 in a PRC article

Influence of uncertainties in various input on the prediction from the standard solar model (A. Serenelli et al., PRD87(2013)043001)

TABLE III. Estimated 1σ uncertainties in solar (from Bahcall, Serenelli, and Basu [14] and nuclear physics (from Adelberger *et al.* [5]) uncertainties, and their influence on flux predictions, computed from the partial derivatives of Table I.

β_j	Value	$\frac{\Delta\beta_j}{\beta_j}$ (%)	$\frac{\Delta\phi(^8\text{B})}{\phi(^8\text{B})}$ (%)	$\frac{\Delta\phi(^7\text{Be})}{\phi(^7\text{Be})}$ (%)	$\frac{\Delta\phi(^{13}\text{N})}{\phi(^{13}\text{N})}$ (%)	$\frac{\Delta\phi(^{15}\text{O})}{\phi(^{15}\text{O})}$ (%)
L_\odot	3.842×10^{33} ergs/s	0.4	2.8	1.4	1.8	2.4
Opacity	1.0	2.5	6.5	3.0	3.7	5.1
Age	4.57 Gyr	0.44	0.59	0.33	0.41	0.60
Diffusion	1.0	15.0	4.0	1.9	5.1	5.7
p + p	$(4.01 \pm 0.04) \times 10^{-25}$ MeV b	1.0	2.6	1.0	2.2	2.9
$^3\text{He} + ^3\text{He}$	(5.21 ± 0.27) MeV b	5.2	2.1	2.2	0.16	0.12
$^3\text{He} + ^4\text{He}$	(0.56 ± 0.03) MeV b	5.4	4.3	4.6	0.33	0.28
p + ^7Be	(20.8 ± 1.6) eV b	7.7	7.7	0.0	0.0	0.0
e + ^7Be		2.0	2.0	0.0	0.0	0.0
p + ^{14}N	(1.66 ± 0.12) keV b	7.5	0.05	0.0	5.6	7.5

Accurate determination of the S(0)-factor for $^3\text{He}+^4\text{He}\rightarrow^7\text{Be}$ is desired.



Digitization – Comment on X4 in a PRC article (cont)

R-matrix analysis by R.J.deBoer et al. (PRC90(2014)035804)

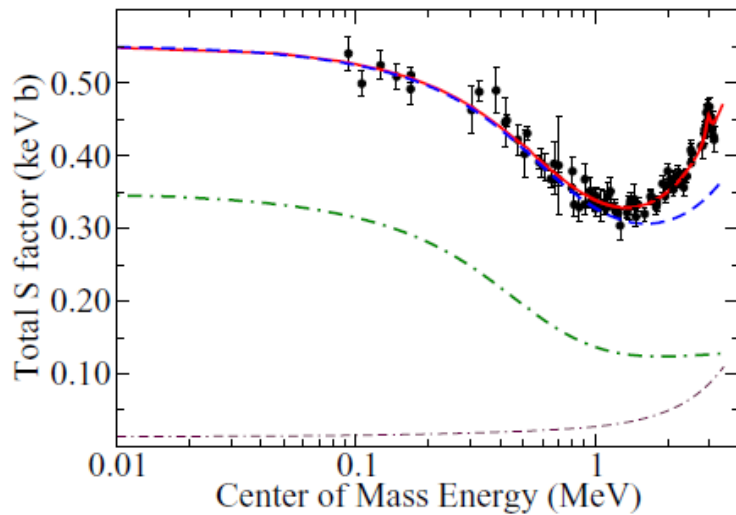


FIG. 4. (Color online) Different *R*-matrix components used for the fit to the ${}^3\text{He}(\alpha, \gamma){}^7\text{Be}$ cross section. The data points are all recent

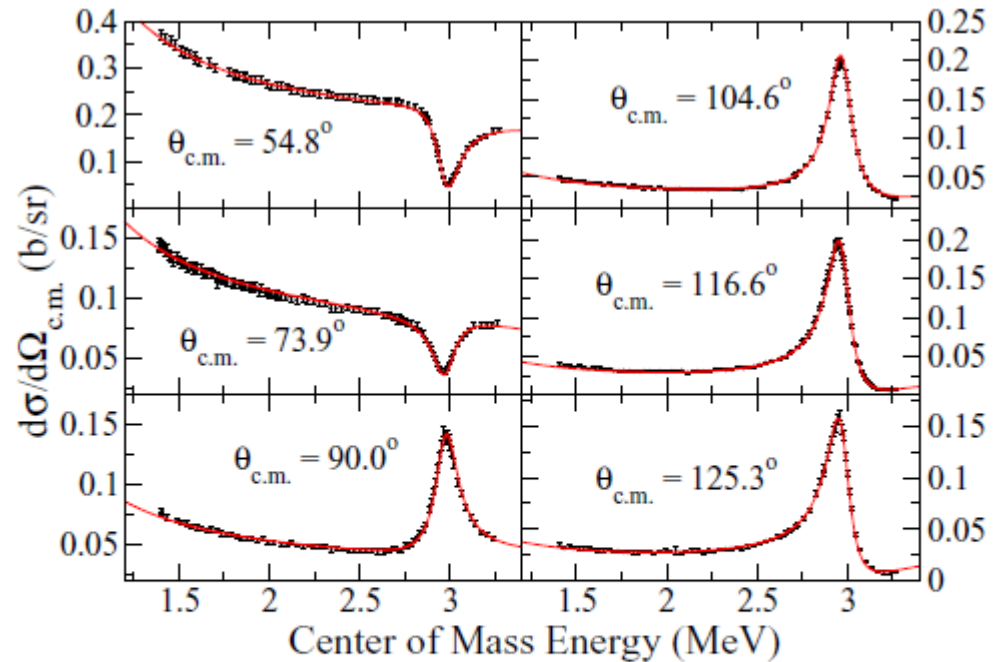
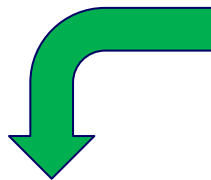


FIG. 8. (Color online) Example excitation curves representative of the fit to the ${}^3\text{He}(\alpha, \alpha){}^3\text{He}$ data of Ref. [34] performed simultaneously with the capture data. The data have been digitized from Fig. 2 of that work by the authors.



²A digitization of this data was also available on EXFOR [53]. It was found that this digitization had a significant offset in the energy scale of several of the excitation curves. !!

[53] V. Zerkin, <http://www-nds.iaea.org/exfor/exfor.htm>



Digitization – Comment on X4 in a PRC article (cont)

Digitized values in EXFOR on the original figure

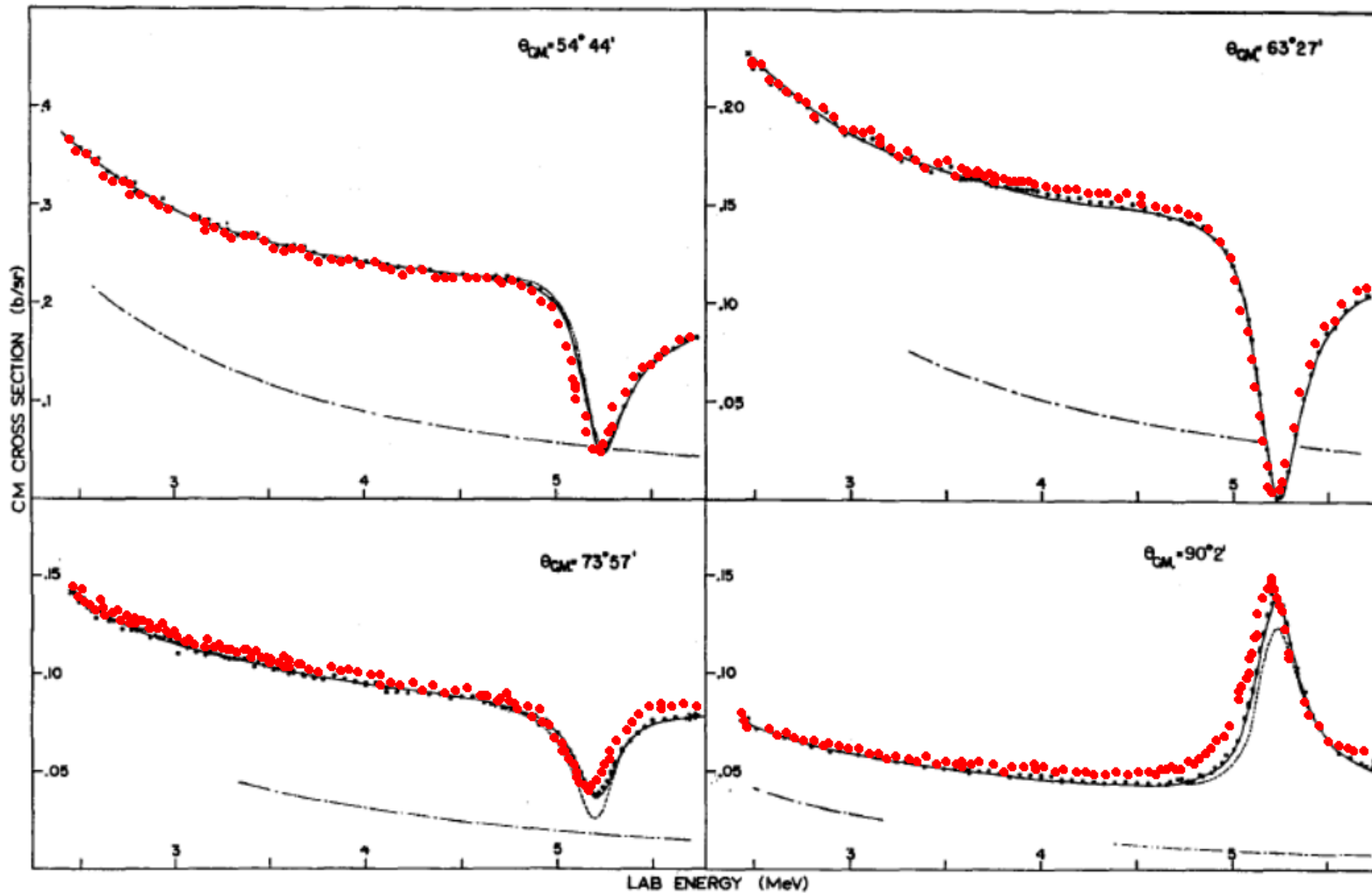
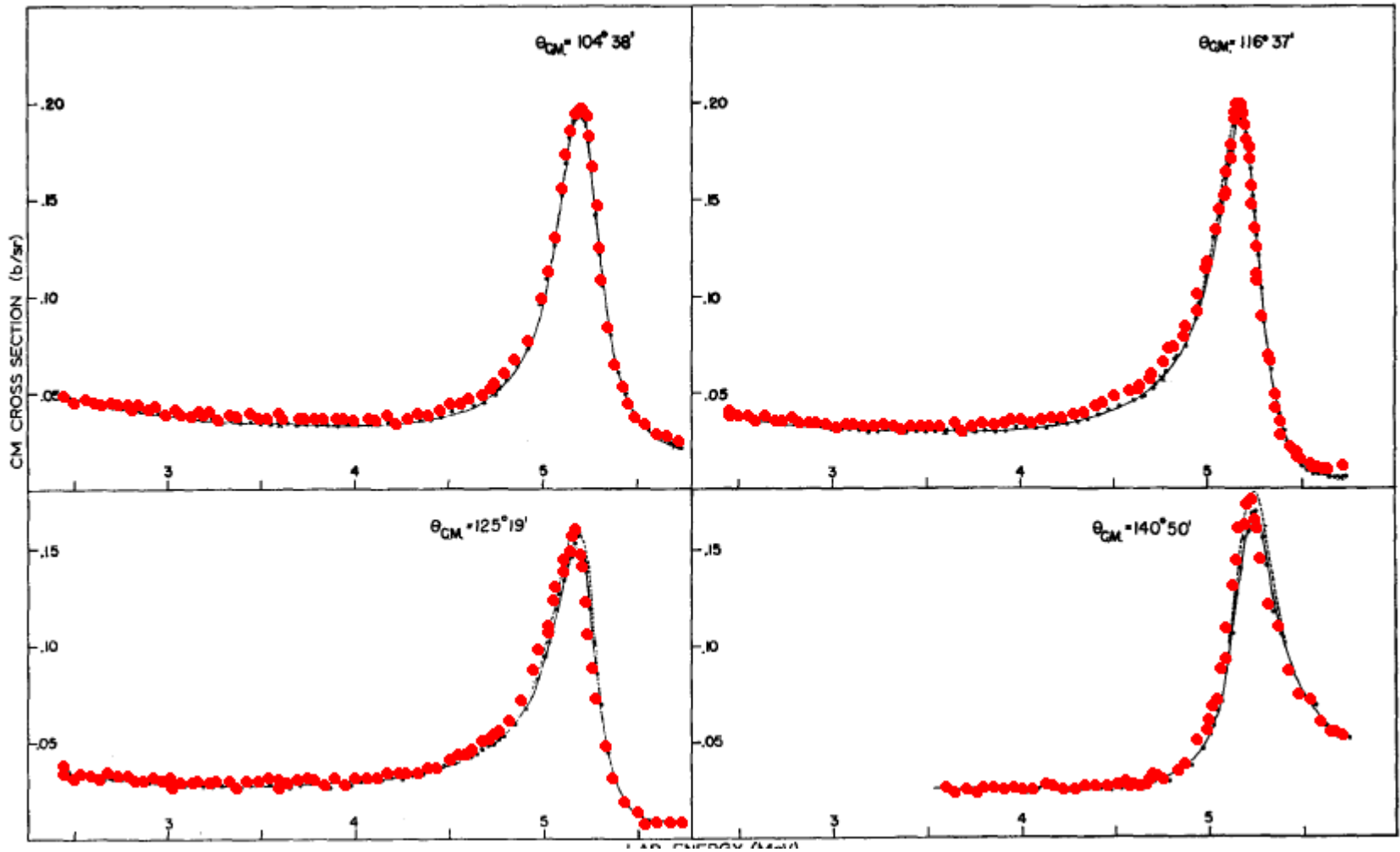


Fig. 2(a).



Digitization – Comment on X4 in a PRC article (cont)

Digitized values in EXFOR on the original figure (cont)



DECAY-DATA - $T_{1/2}$ vs Isomeric Flag

- ~1200 strange relations between the nuclide code and $T_{1/2}$ were detected by my tool (More than 50% deviation in $T_{1/2}$ from wallet cards.)
- **Initial checking:** Sveta Babykina checked each case against the original article, and made a proposal of correction. (completed)
- **Second checking:** Then currently I am checking her comment one by one. I have finished it for ~800 cases.



DECAY-DATA - $T_{1/2}$ vs Isomeric Flag (cont)

Examples of straightforward correction

- Trivial mistake by compiler (*e.g.*, “53.5 day” in article but “53.5HR” by compiler) .
- Change in the level order (*e.g.*, 5 hr g.s. and 70 min m.s. of ^{110}In . See also F.Tarkanyi et al., NIMB245(2006)379 about the history).

Examples of non-straightforward correction

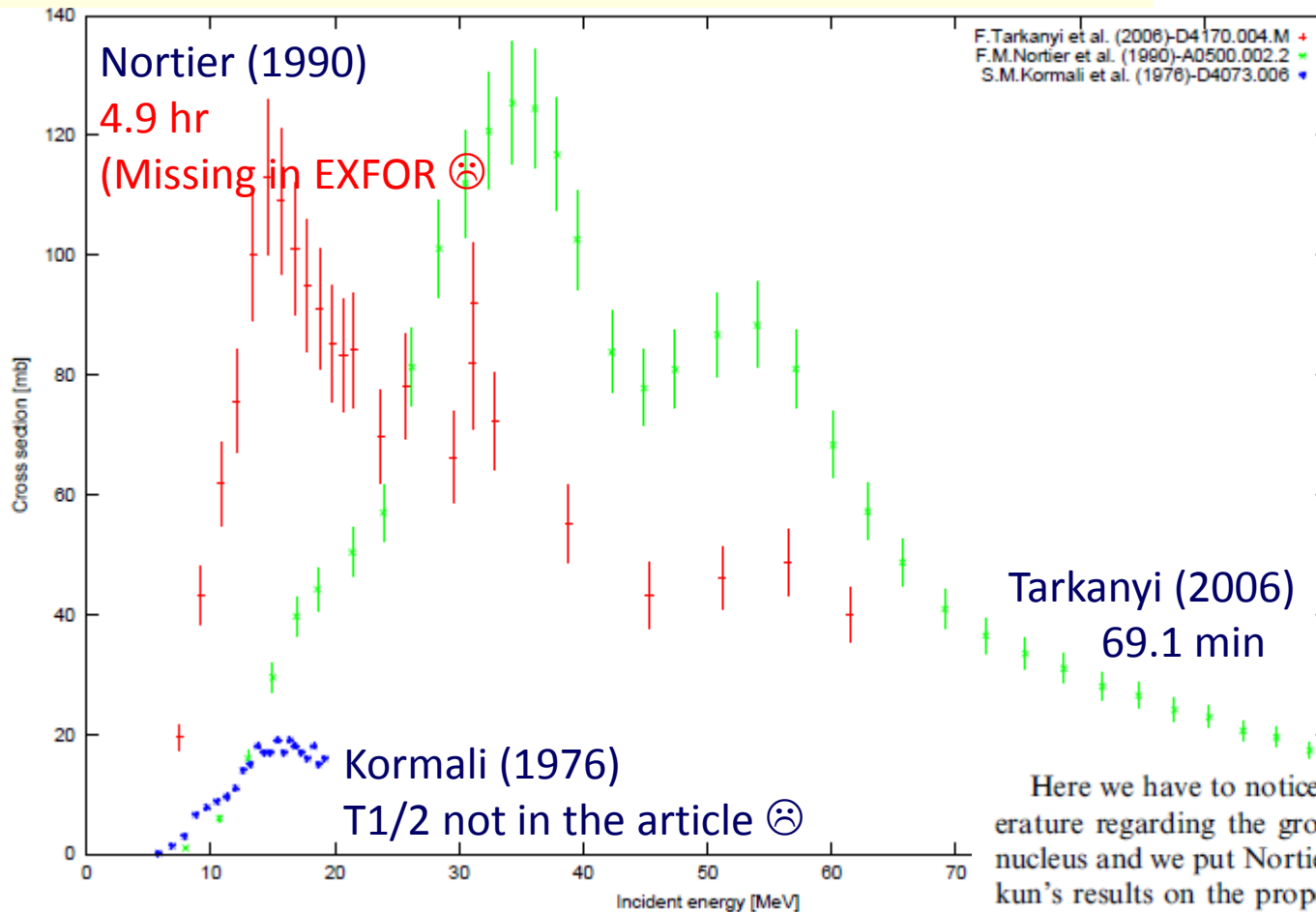
- Strange $T_{1/2}$ in the original article without detailed decay radiation information.
- Assignment of isomeric flag when level ordering of g.s. and m.s. uncertain (*e.g.*, 17 sec and 6 min state of ^{108}Rh).

What should be used? -A? -B? -X?



DECAY-DATA - $T_{1/2}$ vs Isomeric Flag (cont)

(48-CD-0 (P, X) 49-IN-110-M, , SIG) in EXFOR



My program does not detect this case because the compiler did not give DECAY-DATA. (D. Steyn informed me.)

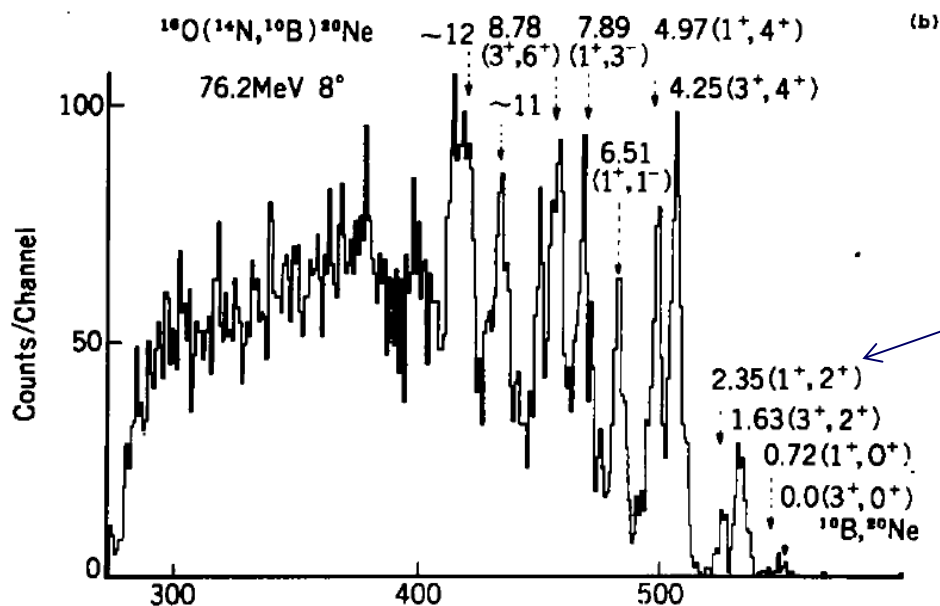
Here we have to notice that there is confusion in the literature regarding the ground and metastable state of this nucleus and we put Nortier's, Kormali's, Otozai's and Ska-kun's results on the proper category if it was necessary.

F.Tarkanyi et al., NIMB245(2006)379



Level Energies in Heavy-Ion Binary Reactions

$^{16}\text{O}(^{14}\text{B},^{10}\text{B})^{20}\text{Ne}$ energy spectrum (T. Motobayashi et al., NPA331(1979)193)



“2.35 MeV ($^{10}\text{B},^{20}\text{Ne}$)= $(1^+, 2^+)$ ”
 $\rightarrow E_x = (0.72 \text{ MeV}, 1.63 \text{ MeV})$.

The two body kinematics gives us the sum of excitation energies of two nuclides in the exit channel.

E-LVL1 and E-LVL2 are expected when partial data are given for a heavy-ion binary reaction.



Alternative (Interdependent) Results

Interdependent Data

Different results for **the same quantity** obtained in the same experiment by two different methods of analysis may be coded in the same subentry.

Such data may also be entered in separate subentries, in which case, the subentries should be linked to each other using STATUS code **COREL**. (LEXFOR S.21).

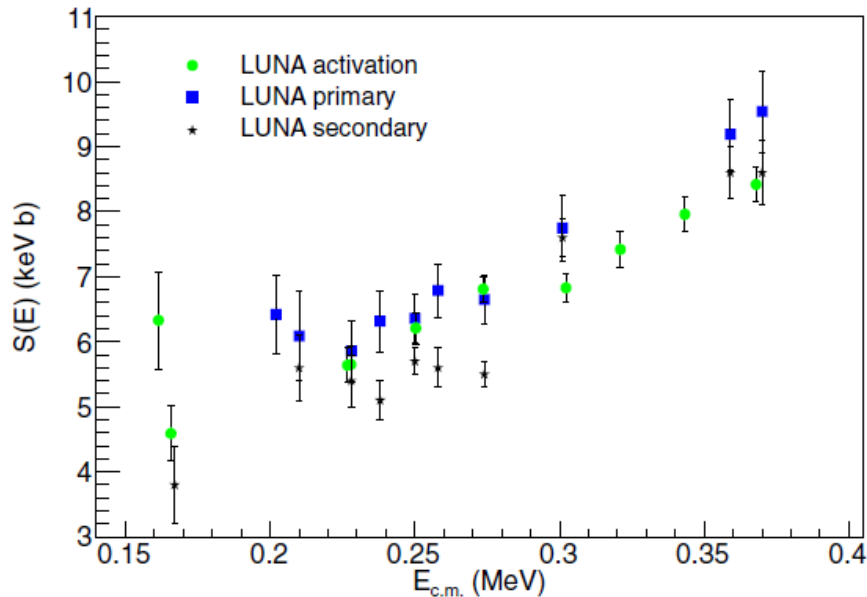
Examples:

- Two data sets obtained by off- and on-line analysis.
- Two data sets from two flight paths.
- 0th order (cross section) and higher order fitting coefficients
(an example of different but interdependent quantities)



Alternative (Interdependent) Results (cont)

$^{17}\text{O}(p,\gamma)^{18}\text{F}$ S-factor from off-line (green) and on-line (blue, black) analysis
(A. Di Leva et al., PRC89(2013)015803)



These 3 data sets may be compiled in

- the same subentry by the multiple reaction formalism,
- or
- different subentries linked by STATUS=COREL each other.

Do *not* distinguish these data sets by **FLAG!**

Each data set must be differentiated by free text (e.g., “activation”, “prompt gamma”) otherwise it looks like duplication.



Alternative (Interdependent) Results (cont)

Two data sets reported in the same article and compiled in two separate entries are *not* always interdependent.

Example:

Neutron data and photonuclear data compiled in two entries reported in the same article are not always interdependent (i.e., linked not by STAUTS=COREL but by REL-REF=0).

Compilation in separate entries

If separate experiments from different service areas with clearly separated results are reported in the same paper, the results should be compiled in separate entries. This applies also if the data were measured at one laboratory, and, subsequently, analyzed at another laboratory and the laboratories are in different areas. The entries may be linked using the STATUS code COREL; see Status (Interdependent Data).

The separation is obligatory if data for different projectile types (neutron, charged particle, photon) are reported in the same publication.

In all such cases cross references to the other entry must be given.

This must be done by
REL-REF=0.



Keywords of Deleted Entries

Deletion of entries

... Not all keywords must be retained; in general, the following information-identifier keywords must be included (left) in the BIB section: **REFERENCE, TITLE, AUTHOR, INSTITUTE, and HISTORY.** (EXFOR Formats 8.2)

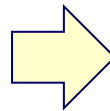
Namely, decision on the rest of the keywords is up to the compiler. It could be however better to delete unnecessary keywords to avoid future updates (due to mistakes, new rules, new dictionaries etc.).



Keywords of Deleted Entries (cont)

```

SUBENT      00143001  20120521
BIB          15      40
TITLE       Isospin dependence of the 65 MeV proton optical
            potential in f-p shell nuclei.
AUTHOR      (T.Noro,H.Sakaguchi,M.Nakamura,K.Hatanaka,F.Ohtani,
            H.Sakamoto,S.Kobayashi)
INSTITUTE   (2JPNKTO)
            (2JPNOSA)
REFERENCE   (J,NP/A,366,189,1981)
PART-DET    (P)
DETECTOR    (HPGE) Elastically scattered protons were detected by
...
FACILITY    (CYCLO,2JPNOSA)
METHOD      (SITA,EXTB,BCINT). The 65 MeV polarized proton beam.
...
REL-REF     (I,E0243001,S.Kato+,J,NIM,169,589,1980)
...
INC-SPECT   EN-RSL . the overall FWHM energy resolution.
ERR-ANALYS (DATA-ERR) The sum of the statistical errors and
...
            (ANG-ERR-D). Data point reader uncertainty.
            (ERR-DIG). Data point reader uncertainty.
...
ADD-RES     (COMP).Optical model using 'MAGALI' code.
...
STATUS      (CURVE) by CAJaD from fig.1 (a,b) of NP/A,366,189,1981
...
ENDBIB      40      0
COMMON      5      3
EN          EN-RSL  ANG-RSL  DATA-ERR  ANG-ERR-D
MEV         MEV    ADEG     PER-CENT  ADEG
65.         0.2    0.05    1.8      0.19
    
```



```

SUBENT      00143001  20120521
BIB          15      40
TITLE       Isospin dependence of the 65 MeV proton optical
            potential in f-p shell nuclei.
AUTHOR      (T.Noro,H.Sakaguchi,M.Nakamura,K.Hatanaka,F.Ohtani,
            H.Sakamoto,S.Kobayashi)
INSTITUTE   (2JPNKTO,2JPNOSA)
REFERENCE   (J,NP/A,366,189,1981)
FACILITY    (CYCLO,2JPNOSA)
STATUS      (CURVE) by CAJaD from fig.1 (a,b) of NP/A,366,189,1981
HISTORY     (19950625C)
            (19950628U)
            (20120521D) SD: Entry deleted. Duplication with E0249.
            Updated to new date formats,lower case; corrected
            according to last EXFOR rules and Dict.
            Year of ref. corrected.
ENDBIB      40      0
NOCOMMON
    
```

Here FACILITY and STATUS are kept
In addition to the minimum keywords
required in LEXFOR.



Free Text – *Be short and precise!*

Free Text

(See also EXFOR Formats Manual Chapter 3).

Be short and precise!

Lengthy free text information may hide essential free text information. The compiler should not do “copy and paste” and should identify key information to be kept as free text.



Free Text – *Be short and precise!* (cont)

How to make free text more visible?

- **Enter the free text under the keyword and code to which it pertains.** (from LEXFOR, underlined part is addition proposed by NO)
- **Do not expand coded information by free text in general.**

“In general, the contents of the coded information should not be repeated in free text, since the coded information is either self-explanatory, as in the case of AUTHOR, or the codes are designed for machine processing.” (from LEXFOR).

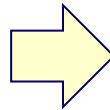
N.B. This may contradict with the “Expansions of these codes may be used, at the compiler's discretion, embedded in free text.” (EXFOR Formats 3.3).
- **Use coded information instead of free text when possible.**



Free Text – *Be short and precise!* (cont)

(ACTIV, EXTB, STTA, GSPEC, MOSEP)

Excitation function was measured via the activation technique using stacked foil targets. Six stacks were irradiated at 16.0, 20.7 And 26.6 MeV. Irradiation time were between 0.5 and 2 hours, the beam current was 100 to 200 Na. The beam energy was measured directly by measuring the time between the beam bunches in Juelich, and was determined from the extraction radius and the cyclotron frequency in Debrecen. For monitoring the beam Ti and Cu foils were used.



(ACTIV) Irradiated for 0.5 to 2 hours with the beam current was 100 to 200 nA.

The beam energy was measured directly by measuring the time between the beam bunches in juelich, and was determined from the extraction radius and the cyclotron frequency in Debrecen.

(MOSEP) Ti and Cu foils used for monitoring the beam.

(STTA) Six stacks were irradiated at 16.0, 20.7 and 26.6 MeV.

(EXTB, GSPEC)

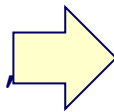


Free Text – *Be short and precise!* (cont)

(2ITYBAU) Istituto Nazionale di Fisica Nucleare (INFN), Bari, Italy. G.Tagliente, corresponding author, Email = guisepe.tagliente@ba.infn.it; N.Colonna, S.Marrone, R.Terlizzi

(2ITYTRI) Istituto Nazionale di Fisica Nucleare (INFN), Trieste, Italy. K.Fujii, P.M.Milazzo, U.Abbondanno, F.Belloni, C.Moreau

(2FR SAC) CEA/Saclay-DSM/DAPNIA, Gif-sur-Yvette, France. G.Aerts, S.Andriamonje, E.Berthoumieux, W.Dridi, F.Gunsing, J.Pancin, L.Perrot, A.Plukis

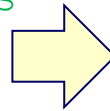


(2ITYBAU, 2ITYTRI, 2FR SAC)



Free Text – *Be short and precise!* (cont)

Nuclear data were taken from E. Browne, R.B.Firestone, Table of radioactive isotopes, ed. V.S.Shirley, Wiley, 1986, New York. To calculate the particles energies in the foils Ziegler's stopping table was used. (J.F.Ziegler, the stopping and ranges of ions in matter, vol 3. Pergamon, New York, 1977)



(R,,J.F.Ziegler,B,ANDERSEN,3,1977)

Stopping power given

(R,,E.Browne+,B,BROWNE,,1986)

Decay data given



ERR-ANALYS – source to be described

The Formats Manual introduces

“ERR-ANALYS. Explains the **sources** of uncertainties and the values given in the COMMON or DATA sections under data headings of the type ERR- or -ERR.”

where sources does NOT mean where the compiler found the uncertainties BUT what **types of error sources** are considered (e.g., counting statistics, normalization).



ERR-ANALYS – source to be described (cont)

Example (“source” is misunderstood by the compiler):

ERR-ANALYS	(DATA-ERR) The uncertainty is reported by authors on figure
------------	---

must be

ERR-ANALYS	(DATA-ERR) No information on source of uncertainties
------------	--

when there is no information.



ERR-ANALYS – Should we explain ERR-DIG?

Example (three error fields are given):

ERR-ANALYS	(EN-ERR-DIG) Digitization error of EN (ERR-DIG) Digitization error of DATA (DATA-ERR) Not specified. Error bars digitized.
-------------------	---

could be simplified to

ERR-ANALYS	(DATA-ERR) No information on source of uncertainties
-------------------	---

and leave further explanation to output systems, e.g., on X4+:

```
COMMON          2          1          12
                #Legend: 2 x 1 x 12 : data columns * lines * column width
                #EN-ERR-DIG   Digitizing error of incident particle energy PER-CENT per-cent
                #ERR-DIG     Digitizing error (of DATA) PER-CENT per-cent
                #/Legend
EN-ERR-DIG      ERR-DIG
PER-CENT        PER-CENT
2.19           .95
ENDCOMMON
```



HISTORY

NRDC2014 C28:

All important alterations must be described in each affected data subentry in addition to a short summary (e.g., subentry numbers) in the common (001) subentry.

NRDC2014 A12 (to me):

Delete the following footnote in the LEXFOR entry “History”:
Compilers are urged to document all changes under HISTORY.

Make important alterations more visible!

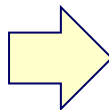


HISTORY (cont)

```

ENTRY          X1216   20130208
SUBENT         X1216001 20130208
BIB            9       17
...
HISTORY (19970404T) + + Converted and updated at DKE + +
(20130208A) N.N. Upper -> lower case correction.
Dates were corrected for 4-digits year.
REACTION SF4 in Subent 002 was corrected
95-AM-240-M -> 95-AM-240-L according to the comment of
N.Otsuka (NDS, IAEA) .
DATA 2, DATA 3 were added.
ENDBIB          17       0
NOCOMMON        0       0
ENDSUBENT       20       0
SUBENT          41216002 20130208
BIB             5       10
REACTION 1 (95-AM-241 (N,2N) 95-AM-240-L,,SIG)
2 (95-AM-241 (N,2N) 95-AM-240-G,,SIG)
3 (95-AM-241 (N,2N) 95-AM-240-L/G,,SIG/RAT)
DECAY-DATA      Are not given in the article.
Supposed as : 95-AM-240-L,0.9MSEC
REFERENCE (W,PLEVE,1966)Private communication of V.P.Zommer,1966
to A.A.Pleve,S.M.Polikanov+ .
STATUS (TABLE) Table 1 of J,YF,6,488,1967 .
(APRVD) Private communication to V.P.Zommer,1966.
HISTORY (19970404T) + + Converted from SUBENT 80342002 + +
ENDBIB

```



```

ENTRY          X1216   20130208
SUBENT         X1216001 20130208
BIB            9       17
...
HISTORY (19970404T) + + Converted and updated at DKE + +
(20130208A) N.N. Major revision in 002.
ENDBIB          17       0
NOCOMMON        0       0
ENDSUBENT       20       0
SUBENT          41216002 20130208
BIB             5       10
REACTION 1 (95-AM-241 (N,2N) 95-AM-240-L,,SIG)
2 (95-AM-241 (N,2N) 95-AM-240-G,,SIG)
3 (95-AM-241 (N,2N) 95-AM-240-L/G,,SIG/RAT)
DECAY-DATA      Are not given in the article.
Supposed as : 95-AM-240-L,0.9MSEC
REFERENCE (W,PLEVE,1966)Private communication of V.P.Zommer,1966
to A.A.Pleve,S.M.Polikanov+ .
STATUS (TABLE) Table 1 of J,YF,6,488,1967 .
(APRVD) Private communication to V.P.Zommer,1966.
HISTORY (19970404T) + + Converted from SUBENT 80342002 + +
(20130208A) N.N. REACITON(SF4): -M -> -L also g.s.
production and isomeric ratio data added.
ENDBIB

```

I personally do not want to see “ 4 digits year”, “upper -> lower” especially when more important alteration is done.



Digitization – Guideline of Expression

Keep consistency for the number of digits between the digitized values and uncertainties.

Example:

DATA

EN	DATA	DATA-ERR
MEV	MB	MB
14.1	12. <u>34</u>	2. <u>34</u>
14.3	12. <u>3</u>	2. <u>3</u>
14.5	1. <u>234</u> E+01	0. <u>234</u> E+01
14.6	1. <u>23</u> E+01	0. <u>23</u> E+01

...



Digitization – Guideline of Expression (cont)

Use the fixed and floating decimal point expression for the numbers digitized from linear and logarithmic scale, respectively.

Example:

12.345

(a value digitized from linear scale)

1.2345E+02

(a value digitized from logarithmic scale)



Digitization – Guideline of Expression (cont)

Digitization accuracy may be given in the absolute unit (e.g., ADEG) or relative unit (e.g., PER-CENT) for the numbers digitized from linear and logarithmic scale, respectively.

Example:

COMMON			
ANG-ERR-D	ERR-DIG		
ADEG	PER-CENT		
<u>0.12</u>	1.2		
ENDCOMMON			
DATA			
ANG-CM	DATA	DATA-ERR	
ADEG	MB	MB	
<u>5.67</u>	3.456E+02	0.234E+02	
<u>12.31</u>	2.345E+02	0.123E+02	

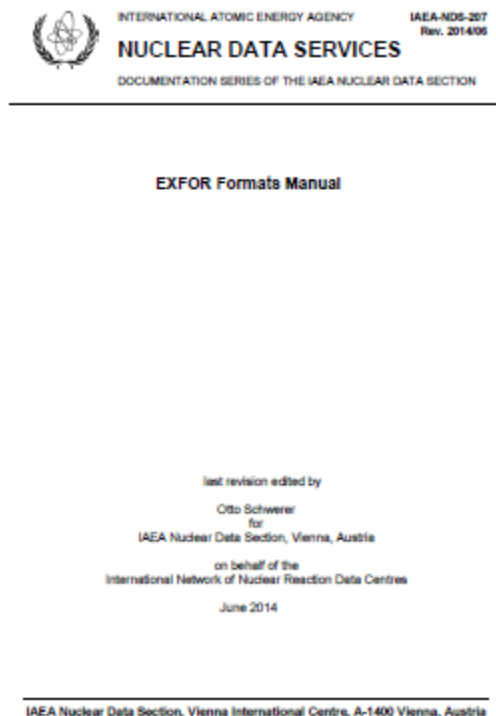
This example also emphasizes consistency for the number of digits between digitization uncertainty and digitized value for ANG.

...

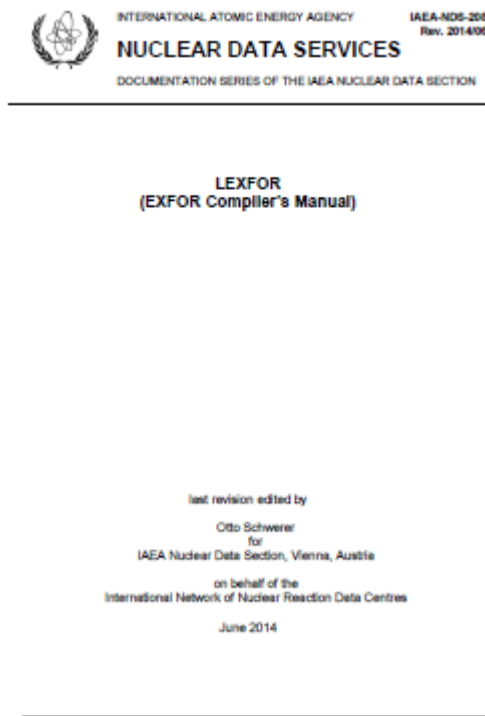


Updated manuals (Formats, LEXFOR, Dictionary)

- Revised manuals (Formats, LEXFOR and Dictionary) have been drafted by Otto in June 2014. It now waits my reviews ☹️



IAEA-NDS-207 Rev. 2014/06



IAEA-NDS-208 Rev. 2014/06



IAEA-NDS-213 Rev. 2014/06

