Nuclear Data Section
International Atomic Energy Agency
P.O.Box 100, A-1400 Vienna, Austria

Memo CP-D/627

Date: 20 March 2010
To: Distribution
From: N. Otsuka. E. Dupont
Subject: **Automatic test of EXFOR with TALYS**

As a part of activity of WPEC sg30, Arjan Koning (NRG Petten) created a complete nuclear reaction database SALTY by blind TALYS calculation, and compared the database with EXFOR for the following reaction/quantity:

Projectiles: γ, n, p, d, t, ^{3}He, α
Targets: all stable isotopes with $9 \leq Z \leq 83$
Inc. energy: from thermal energies up to 200 MeV
Reaction: total, elastic, non-elastic, exclusive partial cross sections (defined by the ENDF MT scheme), and residual production cross sections.

The deviation of the SALTY data from EXFOR data were evaluated by the following 4 averaged deviation factors:

Rolf Michel's f-factor
$$F = 10^{\sqrt{\frac{1}{N}\sum_{i=1}^{N}\left[\log\left(\sigma_S^i / \sigma_E^i\right)\right]^2}}$$

C/E value
$$R = \frac{1}{N}\sum_{i=1}^{N}\frac{\sigma_S^i}{\sigma_E^i}$$

Chi-square
$$\chi^2 = \frac{1}{N}\sum_{i=1}^{N}\left(\frac{\sigma_S^i - \sigma_E^i}{\Delta\sigma_E^i}\right)^2$$

Absolute deviation
$$\Delta = \frac{1}{N}\sum_{i=1}^{N}\left|\sigma_S^i - \sigma_E^i\right|$$

and compiled in one ASCII file (x4.sort), which was sent to NDS with the associated documentation (appended to this memo).

Then suspicious EXFOR subentries potentially involved in coding mistake (e.g. B $\leftrightarrow$ MB) were selected by the NEA Data Bank using the following criteria (assuming that calculated value could be wrong by up to a factor of 2)

$5 \times 10^{-4} < R < 2 \times 10^{-3}$ or $5 \times 10^{+2} < R < 2 \times 10^{+3}$ or $500 < F < 2000$

This selection of EXFOR subentries was further filtered at the NEA Data Bank by comparison with other experimental and evaluated data in order to eliminate false alarm, X4toC4 issue, and known errors. The result is summarized in Table 1. During this visual inspection, some additional outliers were found (outside the F or R selection range).

Finally 37 suspicious data sets were checked with original articles by NDS and real coding mistakes were found in 25 data sets. For several cases, NDS asked questions to authors, and Prof. R. Michel (Uni. Hannover) and T. Otsuki (Tohoku Univ.) answered us quickly.

Please find proposed corrections in "Report to WPEC SG30" appended to this memo. A short summary is also shown in the NRDC webpage:
http://www-nds.iaea.org/nrdc/error/exfor_err3.html.
Plots prepared by the NEA Data Bank were also added to the web page.

Table 1: Deviation factors of suspicious data sets after filtering of the list provided by A. Koning

# EXFOR	E-min (eV)	E-max (eV)	F	R	χ^2	Δ
10492.008	8.70E-01	3.97E+00	332.	517.	1.483E+07	2.418E+03
12244.002	2.35E-08	2.35E-08	695.	1.439E-03	5.05	8.987E+04
12758.006	3.00E-02	3.00E-02	887.	1.127E-03	395.	8.940E+04
13547.004	1.50E+00	3.50E+00	1.226E+03	8.626E-04	31.9	146.
13783.004	2.53E-08	2.53E-08	521.	1.921E-03	99.6	1.397E+07
14075.004	3.00E+00	4.00E+00	689.	4.032E-03	108.	91.0
21486.002	2.53E-08	2.53E-08	749.	1.335E-03	12.6	3.196E+04
22347.006	1.35E+01	1.47E+01	1.438E+03	1.442E+03	1.146E+08	1.627E+03
22445.002.2	3.75E-02	3.75E-02	1.138E+03	8.785E-04	178.	187.
22873.003	3.65E-03	5.25E-02	1.190E+03	1.193E+03	6.020E+08	7.740E+03
31543.006	1.40E+01	1.40E+01	1.381E+03	7.240E-04	18.8	6.50
31602.002	2.53E-08	2.53E-08	1.312E+03	1.312E+03	9.536E+08	556.
32205.019	1.45E+01	1.45E+01	653.	1.531E-03	16.0	0.759
40244.048	4.00E+00	4.00E+00	1.042E+03	1.042E+03	9.533E+08	1.85
40244.049	4.00E+00	4.00E+00	521.	521.	2.676E+07	0.931
40336.102	2.50E+00	4.00E+00	821.	1.240E-03	0.00	749.
A0401.002	3.97E+01	1.10E+01	1.113E+05	8.529E-04	24.6	2.77
A0485.010	4.20E+01	1.03E+02	3.362E+04	1.499E-03	40.3	1.56
O0282.005	5.32E+01	9.80E+01	8.860E+04	1.224E-03	81.1	1.75
C0265.008	4.08E+01	3.56E+01	569.	570.	8.128E+06	0.131
C0703.004.2	7.00E+00	1.10E+01	991.	1.007E+03	2.644E+07	91.6
C1159.003.1	1.92E+01	3.96E+01	89.6	697.	3.742E+09	128.
C1523.004	3.66E+01	3.66E+01	635.	635.	2.129E+08	146.
D0433.002	4.64E+00	2.74E+01	5.858E+05	9.820E-04	44.4	108.
E1411.006	1.20E+01	1.80E+01	5.064E+04	5.683E-04	32.2	366.

Table 2: Summary of checking with articles

Not in error	9
Error (corrected)	2
Error (to be corrected)	23
Not resolved yet	3
Total	**37**

Common remark to centres for all lists from WPEC sg30 activity:
Addition of CRITIQUE may help users even if deviation is not attributed to coding mistake!!

Report to WPEC SG30

Analysis of a selected suspicious data from Arjan Koning's list (x4.sort) (Draft Ver. 2010-03-20 by Naohiko)

Source:

Table: Table of data is given in the reference.

Curve: Plot of data is given in the reference.

SCSRS: Data translated from the SCISRS library.

Author: Data received from authors.

Trans: EXFOR transmission number if corrected

Subentry	Reference	Reaction	Comments (AK+ED)	Source	Error?	Trans	Comments (NO)
10492.008	J,NSE,67,34,1978	24-CR-0(N,INL)24-CR-54,PAR,SIG	30 times too low	Author	Yes		**SF4: 24-CR-54→24-CR-0** or **SF1: 24-CR-0 → 24-CR-54** **SF8: Add A** a (^{54}Cr)=2.4%. Similar comments are applied to **002, 004, 006** (and **014**?).
12244.002	W,HALDAR,1953	78-PT-192(N,G)78-PT-193-M,,SIG	10 times too large	SCSRS	?		***Checking by NNDC*** (Supported by 31249.009)
12758.006	J,PR/C,29,2126,1984	82-PB-204(N,G)82-PB-205,,SIG,,MXW	1000 times too large	Table	Yes		**DATA(-ERR): B → MB** In addition, EN-MEAN → KT DATA-ERR→ERR-T Add ERR-S=0.2%. Note that +/- 5.5 mb is given in p2134 of the article. But +/- 4.5 mb in the abstract is more consistent with the description in IV Discussion.

13547.004	J,JP/G,19,655,1993	21-SC-45(N,INL)21-SC-45,PAR,SIG	wrong level energy (1000 times too low)	Author	Yes		**E-EXC(-ERR): KEV → MEV**
13783.004	C,99SANTA,,111,1999	64-GD-148(N,G)64-GD-149,,SIG,,MXW	100 times too large	Table	?		Superseded by 14113.002 ? (Declared as a preliminary result in M.G. Rios *et al*., J,PR/C,74,044302,2006)
14075.004	J,NP/A,500,43,1989	40-ZR-96(N,INL)40-ZR-96,PAR,SIG	5 times too large? (1st level only)	Table	Yes		**Excitation energies for E_n=3.0 MeV and 3.5 MeV (except for last 3 levels) must be corrected. Also 12 mb → 2 mb for the 3483 keV level at E_n=4.0 MeV.**
14113.002	J,PR/C,74,044302,2006	64-GD-148(N,G)64-GD-149,,SIG	100 times too large (see 13783004.png)	Table	No		
21486.002	J,CR,252,3973,1961	10-NE-0(N,G),,SIG	1000 times too large	Table	Yes		**DATA(-ERR): B → MB**
22347.006	S,JAERI-97-004,177,1996	53-I-129(N,2N)53-I-128,,SIG	1000 times too low	Table	Yes		**MB→B (006)** c.f. Fig.2. In addition, - 004-006. STATUS: "Data from main reference" is not applicable. 004-005 and 006 are from S,JAERI-97-C-005,216,1997 (Table 2) and S,JAERI-98-C-003,210,1998 (Table 2). - 002-005: Partial uncertainties are wrong. Information for 002-003 and 004-005 should be taken from S,JAERI-C-97-004, 177, 1996 (Table 2) and S, JAERI-C-97-005, 216, 1997 (Table 3), respectively. - INC-SPECT should be given according to MCNP calculation results explained in p218 of S,JAERI-C-97-005. Contribution of thermal, epithermal. MeV and DT neutron were 30%, negligible, 50% and 20% in 003, and contribution of the thermal neutrons were removed in 005.
22445.002.2	J,PR/C,52,3442,1995	16-S-36(N,G)16-S-37,,SIG,,MXW	1000 times too large? (see also 224450021, 22445003)	Table	Yes		**MB → MICRO-B (002.2 and 003)**
22873.003	C,2004SANTA,,1462,2004	53-I-129(N,TOT),,SIG	1000 times too low	Author	(Yes)	2212	**MB → B**

22965.002	J,PR/C,75,034617,2007	17-CL-36(N,P)16-S-36,,SIG) + (17-CL-36(N,A)15-P-33,,SIG)	2 data sets in the same list??	Author	?		***Waiting authors' answer***
31249.009	J,NP,41,372,1963	78-PT-192(N,G)78-PT-193,,SIG,,SPA	10 times too large (see 12244002.png)	Table	Yes		**SF4: 78-PT-193 → 78-PT-193-M** Identified by KX-rays giving activity of $T_{1/2}$=4.4 d. ($T_{1/2}$= 50 y for g.s.)
31316.010	J,NP,69,153,1965	20-CA-40(N,T)19-K-38,,SIG	1000 times too large	Table	No		Monitor cross section $\sigma(^{56}Fe(n,p)^{56}Mn)$=110 mb @ 14.8 MeV is not bad. No discussion in Z.T.Body *et al.*, C,ANTWER,,368,1982 (EXFOR 30818.003).
31543.006	J,NP/A,722,568,2003	24-CR-54(N,N+P)23-V-53,,SIG	1000 times too large? (threshold)	Table	No		
31602.002	J,NIM/B,266,21,2008	72-HF-179(N,G)72-HF-180-M,,SIG	1000 times too low	Table	Yes		**DATA, ERR-T: MB→B** In addition, **ERR-T: 0.45 → 0.41 (003).**
32205.019	J,NSTS,2,425,2002	57-LA-139(N,N+A)55-CS-135-M,,SIG	1000 times too large? (threshold)	Author	Yes		**MB → MICRO-B** (Confirmed by UkrNDC, 2010-03-16)
40244.048	C,58GENEVA,15,50(2219),1958	23-V-51(N,G)23-V-52,,SIG	1000 times too low	Table	Yes		**DATA(-ERR): MB → B**
40244.049	C,58GENEVA,15,50(2219),1958	25-MN-55(N,G)25-MN-56,,SIG	1000 times too low	Table	Yes		**DATA(-ERR): MB → B (049, 050)** In addition, **DATA → DATA-MAX (002, 009, 011, 017-018, 043, 045, 052, 058-059).** Remove duplication pairs (e.g. 002=043+085)
40336.102	C,58GENEVA,15,18(2030),1958	22-TI-50(N,G)22-TI-51,,SIG	1000 times too large	Table	Yes		**B → MB (102)** In addition, **5.9 +/- 0.0003 mb → 8.6 +/- 0.4 mb (096)**
A0401.002	J,JRN/L,128,403,1988	79-AU-197(A,G)81-TL-201,,SIG,,,EXP	1000 times too large	Table	No		Add DECAY-DATA. Activation cross sections. Their decay data (0.16% and 10.6% for 165.9 keV and 167.4 keV gamma lines are good.). Experimental cross sections of 197Au(n,α)201Tl in EXFOR are scattered each other. The situation is depicted in Fig.3 in J,PAN,70,613,2007 (EXFOR F0858.005).

A0485.010	J,YK,8,17,1990	12-MG-0(P,X)4-BE-7,,SIG,,,EXP	10 times too low? (see also o0282005, C0095008)	Table	No		**REFERENCE: J,YK,8,17,2001→J,VAT/I (1990) no. 8 p.17-24** In addition, STATUS: TABLE must be added (Taken from Table 2). ERR-ANALYSIS: "Data-point reader uncertainty" is probably incorrect. ^{nat}Mg(p,x)^{7}Be cross section in Table 2 is consistent with Fig.9.
C0095.008	J,ARI,41,349,1990	(12-MG-0(P,X)4-BE-7,,SIG)+(8-O-0(P,X)4-BE-7,,SIG)	10 times too high? (see A0485010.png)	Table	Yes?		**SF8: Add FCT ?** Data are for Mg(OH)$_2$. Probably data are normalized to density of the molecule. Data close to twice of σ(^{nat}O(p,x)^{7}Be) data in EXFOR C0401.002 and O0282.004.
C0265.008	J,PR,131,1697,1963	23-V-51(A,N+2A)21-SC-46,,SIG	1000 times too low	Table	Yes		**MICRO-B→ MB (007-009)** **EN → EN-CM (010-013)** **012: First three points should be coded under DATA-MAX.**
C0703.004.2	J,PR,133,B907,1964	28-NI-58(A,P)29-CU-61,,SIG,,,DERIV	1000 times too low	Table	Yes		**MICRO-B→ MB**
C1159.003.1	P,UCRL-115738-5,1,1993	39-Y-89(P,INL)39-Y-89,,SIG	wrong reaction? (threshold is wrong)	Table	Yes		**SF3: INL, EL `→ X** **SF4:** **39-Y-89 → 39-Y-87-M (003.1, 006.1)** **39-Y-89 → 39-Y-87-G (003.2, 006.2)** In addition, DECAY-DATA: $T_{1/2}$ must be given.(c.f. Fig.1) METHOD: Add ACTIV.
C1523.004	J,PR/C,29,764,1984	7-N-14(P,INL)7-N-14,PAR,SIG	1000 times too low? (Partial xs)	Table	No		Partial for the 1st level.
D0433.002	J,RCA,94,795,2006	23-V-0(P,X)23-V-48,,SIG	wrong reaction? (threshold is wrong by 30MeV)	Table	Yes		**SF1: 23-V-0 → 22-TI-0 (002-006)**
E1411.006	J,PR/C,44,1405,1991	94-PU-242(P,F),,SIG	wrong shape? (but only 2 points at threshold)	Author	Yes		**Swap two E_p values (12.0 MeV and 18.0 MeV).**

							Misprint in the data table from authors. (Confirmed by Prof. T. Otsuki, 2010-03-16)
M0041.009	J,NP/A,338,97,1980	73-TA-181(G,ABS),,SIG,,,EXP	wrong reaction? ("ATOMIC CROSS SECTION")	Table	Yes		**Delete or add MSC in SF8 (002-014)** Mainly from atomic interaction.
M0041.013	J,NP/A,338,97,1980	79-AU-197(G,ABS),,SIG,,,EXP	wrong reaction? ("ATOMIC CROSS SECTION")	Table	Yes		(See above)
M0041.014	J,NP/A,338,97,1980	83-BI-209(G,ABS),,SIG,,,EXP	wrong reaction? ("ATOMIC CROSS SECTION")	Table	Yes		(See above)
M0188.007	J,NP/A,446,229(C),1985	13-AL-27(G,ABS),,SIG,,FCT,EVAL	27 times too low ("XS WAS MULTIPLIED BY 1/A")	Author	No		FCT (times a factor) is indicated in SF8. In addition, this is not an experimental data set.
M0380.003	J,JP/G,19,805,1993	73-TA-181(G,ABS),,SIG,,,EXP	1000 times too low	Table	(Yes)	M051	MICRO-B → MB (003, 005, 007) But they are not authors' experimental data and have already deleted.
M0638.008	J,PR/C,65,044622,2002	82-PB-0(G,F),,SIG,,FCT	208 times too low ("XS WAS MULTIPLIED BY 1/A")	Table	No		**DATA-ERR → ERR-S (008-013)** FCT (times a factor) is indicated in SF8.
O0276.105	J,NIM/B,129,153,1997	28-NI-0(P,X)24-CR-51,,SIG,,,EXP	xs value is wrong at EN = 126 MeV	Author	Yes		**0.037 mb → 37.0 mb @ 126 MeV** (Confirmed by Prof.R.Michel, 2010-03-17)
O0282.005	J,NIM/B,82,9,1993	12-MG-0(P,X)4-BE-7,,SIG	10 times too low? (see A0485010.png)	Table	No		

Memo CP-D/633

Date:	4 April 2010
To:	Distribution
From:	N. Otsuka. E. Dupont
Subject:	**Automatic test of EXFOR with TALYS (2)**
Reference:	Memo CP-D/627

As a continuation of testing of EXFOR with TALYS, a new list was generated using the following constraints

1. F and (R or $1/R$) > 100
2. For the same reaction (SF2,SF3), target (SF1), product (SF4), and in a similar energy range:
    a) at least 2 independent subentries are available
    b) at most 20% (or $1/n$ with $n < 10$) of these subentries satisfy criteria 1
3. The following data are excluded:
    a) SF8=RAW or SF8=FCT (not to be compared with evaluated/calculated cross sections)
    b) SF8=MXW with $kT = 25.3$ meV (in C4) because part of these data are now incorrectly converted from EXFOR data with $kT\sim30$ keV (stellar temperature spectra).
    c) SF5=PAR (choice of the excited state to be compared is ambiguous)

Finally 12 suspicious data sets (not yet reported) were checked with original articles by NDS and 8 real coding mistakes were found in data sets.

Please find proposed corrections in "Report to WPEC SG30" appended to this memo. A short summary is also shown in the NRDC webpage:
http://www-nds.iaea.org/nrdc/error/exfor_err3.html.
Plots prepared by the NEA Data Bank were also added to the web page.

Common remark for action to the lists from WPEC SG30 activity:
1. Occasionally additional mistakes were found during checking at NDS. It is also written in the comment field.
2. Addition of CRITIQUE may help users even if deviation is not attributed to coding mistake!!

Table 1: Deviation factors of suspicious data sets after filtering of the list provided by A. Koning

# EXFOR	*E*-min (eV)	*E*-max (eV)	*F*	*R*	χ^2	Δ
10835.014	1.48E+01	1.48E+01	405	2.47E-03	107	1.24E+03
11399.003	2.40E-02	2.40E-02	369	2.71E-03	0	14
30079.042	2.40E-02	2.40E-02	1.29E+04	7.74E-05	42.2	6.5
31419.005	7.50E+00	7.50E+00	215	4.66E-03	366	2.54
31556.003	5.00E-10	5.00E-10	9.44E+03	9.44E+03	4.93E+12	3.11E+05
31615.007	1.35E+01	1.48E+01	2.96E+03	2.99E+03	1.2	895
40244.009	2.70E+00	2.70E+00	2.71E+03	2.71E+03	0	14.1
40244.050	4.00E+00	4.00E+00	3.89E+03	3.89E+03	6.04E+07	10.1
41504.002	1.50E-03	1.50E-02	110	121	0	10.2
C0738.002	2.04E+00	4.19E+00	2.06E+03	6.26E+03	8.29E+11	57.9
C0739.008	1.92E+00	4.14E+00	8.50E+03	1.38E+04	3.25E+12	36.1
F0794.003	1.46E+01	1.73E+01	150	150	2.09E+07	258

Table 2: Summary of checking with articles

Not in error	3
Error (corrected)	1
Error (to be corrected)	7
Not resolved yet	1
Total	12

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Report to WPEC SG30

Analysis of a selected suspicious data from Arjan Koning's list (x4.sort) (Draft Ver. 2010-04-03 by Naohiko)

Source:

    Table: Table of data is given in the reference.

    Author: Data received from authors.

Trans: EXFOR transmission number if corrected

Subentry	Reference	Reaction	Comments (AK+ED)	Source	Error?	Trans	Comments (NO)
10835.014	T,SOTHRAS,1977	50-SN-116(N,P)49-IN-116-M2,,SIG	1000 times too large	Author	?		***Checking by NNDC***
11399.003	J,PR,107,504,1957	12-MG-26(N,G)12-MG-27,,SIG	1000 times too large	Table	No		Upper limit (14 mb) given
30079.042	J,PR,152,1055,1966	82-PB-208(N,G)82-PB-209,,SIG	1000 times too large	Table	No		β spectroscopy
31419.005	R,INDC(ARG)-012,1993	22-TI-50(N,A)20-CA-47,,SIG	30 times too large? (threshold)	Table	No		Their decay data (74.9% for 1297.1 keV gamma lines is good.).
31556.003	J,NIM/B,213,32,2004	17-CL-35(N,G)17-CL-36,,SIG	10000 times too low	Table	Yes		**DATA(-ERR): MB → B**
31615.007	J,IPC,77,854,2008	35-BR-79(N,2N)35-BR-78,,SIG	3000 times too low	Table	Yes	3139	**Add EN-ERR in the 2nd column**
40244.009	C,58GENEVA,15,50(2219)1958	28-NI-64(N,G)28-NI-65,,SIG	1000 times too low	Table	Yes		**DATA: MB →B** (See also CP-D/627)
40244.050	C,58GENEVA,15,50(2219)1958	28-NI-64(N,G)28-NI-65,,SIG	1000 times too low	Table	Yes		**DATA(-ERR): MB → B** (See also CP-D/627)
41504.002	R,INDC(CCP)-368,1991	24-CR-0(N,G),,SIG,,AV	1000 times too low	Table	Yes		**DATA: MB → B** **DATA: 0.119 → 0.118 @ 1-2 keV**
C0738.002	T,QIANG,1990	29-CU-65(P,N)30-ZN-65,,SIG	1000 times too low	Table	Yes?		**MICRO-B → MB?** Misprint by authors? (See also CP-D/623)
C0739.008	T,QIANG,1990	29-CU-65(P,N)30-ZN-65,,SIG	1000 times too low	Table	Yes?		**MICRO-B → MB?** Misprint by authors? (See also CP-D/623)
F0794.003	J,NP/A,275,269,1977	9-F-19(P,A)8-O-16,,SIG	20 times too low (or 8-O-16-G production?)	Table	Yes		**Add PAR in SF5 and E-LVL=0.0**