

Illegal repetition of heading

(N. Otsuka, 2023-03-02, Memo CP-D/1070)

Repetition of the same heading may create a trouble during computer processing of EXFOR datasets. For example, codes cannot determine which uncertainty should be used as the total uncertainty if ERR-T is given twice in the COMMON and DATA sections, or given in MB and PER-CENT, and this may create a trouble during construction of covariance etc. “Duplicating HEADER” (<https://nds.iaea.org/exfor-master/x4compil/Errors-main.htm#duplicatingHeader> [1]) summarizes problematic repetitions very well. I reviewed each case against the source article etc., and listed proposed corrections as appended to this memo.

There are typically the following three cases:

1. %-uncertainty in COMMON section, absolute uncertainty in DATA section
2. A value of a running variable in DATA section is repeated in COMMON section
3. The same value is in COMMON and DATA sections.

It is not always trivial to resolve the first case.

Example (21494.009):

Total uncertainty (ERR-T) is given twice in this subentry.

SUBENT	21494009	20160907			
BIB	5	15			
REACTION	((94-PU-241(N,F),,SIG,,MXW)/(92-U-235(N,F),,SIG,,MXW))				
...					
ENDBIB	15				
COMMON	11	6			
ERR-5	ERR-6	ERR-7	ERR-8	ERR-T
PER-CENT	PER-CENT	PER-CENT	PER-CENT	PER-CENT
2.0	0.4	0.4	0.1	2.8
ENDCOMMON	6				
DATA	3	2			
EN-DUMMY	DATA	ERR-T			
EV	NO-DIM	NO-DIM			
0.0253	1.920	0.047			
0.0313	1.966	0.048			
ENDDATA	4				
ENDSUBENT	31				

Before retransmission in TRANS.2187, the subentry looked like:

SUBENT	21494009	810204		
BIB	4	8		
REACTION	((94-PU-241(N,F),,SIG,,MXW)/(92-U-235(N,F),,SIG,,MXW))			
...				
ENDBIB	8			
NOCOMMON	0	0		
DATA	3	2		
EN-DUMMY	RATIO	RATIO-ERR		
EV	ARB-UNITS	ARB-UNITS		
0.0253	1.920	0.047		
0.0313	1.966	0.048		
ENDDATA	4			
ENDSUBENT	17			

We observe the compiler tried to “upgrade” uncertainty coding for retransmission, but it creates a problem.

The point-wise fractional uncertainty is $0.047/1.920=2.5\%$ at 0.0253 eV and $0.048/1.966=2.4\%$ at 0.0313 eV, which disagrees with $ERR-T=2.8\%$ coded in COMMON section. I got the following questions:

1. Is the point-wise uncertainty really total?
2. Is $ERR-T=2.8\%$ in COMMON section applicable to both data points? (It is taken from the error budget table – TABLE IV of C,66PARIS,2,29,1966). An error budget table sometimes provides “typical” uncertainty.

I expect the total uncertainty ($ERR-T$) and statistical uncertainty ($ERR-S$) are not constants of a dataset, and the list appended to this memo proposes deletion of these values in the COMMON section if they are also in the DATA section in general. But I urges each originating centre also review each case (especially case #1) and makes the final decision.

Reference

[1] in the “EXFOR Database Update Error Report” generated by EXFOR-Relational maintenance system (V.Zerkin, 1999-2023)

Addition to WP2023-20 (2023-04-27)

Even for the cases where repletion of the heading is legal, it can be a source of a major trouble during processing by end users. For unresolved secondary energies and masses, I would like to propose code the lower and upper boundaries (e.g., $E-LVL-MIN$ and $E-LVL-MAX$) when possible. There are additional advantages to code ranges instead of the individual numbers:

- This simplifies coding when there are three ore more unresolved values present.
- We do not need to worry about presence of a third energy line (level energy or outgoing particle energy) which is “hidden” between two unresolved energy lines mentioned in the article.

Example:

$E-LVL-MIN$	$E-LVL-MAX$
MEV	MEV
0.077	0.177

rather than

$E-LVL$	$E-LVL$	$E-LVL$
MEV	MEV	MEV
0.077	0.107	0.177

Illegal Repetition of Heading
(based on EXFOR Database Update Error Report 2023-02-13)

Cases

#1: %-uncertainty in COMMON section, absolute uncertainty in DATA section

#2: A value of a running variable in DATA section is repeated in COMMON section

#3: The same value is in COMMON and DATA sections.

Dataset ID#	Heading	Action	Remark
10007.003	DATA-ERR	Delete DATA-ERR=8% in COMMON section.	#1
10007.008	DATA-ERR	Delete DATA-ERR=8% in COMMON section.	#1
10007.013	DATA-ERR	Delete DATA-ERR=8% in COMMON section.	#1
10384.019	DATA-ERR	Delete DATA-ERR=4.0% in COMMON section.	#1
10485.004	EN-ERR	Delete EN-ERR=0.08 MeV in COMMON section.	Wrongly copied from 002.
10785.002	ANG	Delete ANG=125 deg in COMMON section.	#2. Author's letter checked.
10827.017	DATA-ERR	DATA-ERR -> ERR-T in DATA section?	
10875.008	SPIN J	Delete SPIN J=1 in COMMON section.	#2
11319.002	EN-RSL	Delete EN-RSL=50 keV in COMMON section and EN-RSL=0.05 MeV in DATA section (upper limit).	See p.894 (left).
11432.002	DATA-ERR	Delete DATA-ERR=3.5% in DATA section.	#3
11432.003	DATA-ERR	Delete DATA-ERR=2.5% (digitized) in DATA section.	#3
11635.009	STAT-W G	Delete STAT-W G=0.5 in COMMON section.	#3
12220.002	ANG-RSL	Delete ANG-RSL=3.5 deg in DATA section.	#3
12373.010	ANG-RSL	Delete ANG-RSL=6 deg in DATA section.	#3
12688.002	ANG	Delete ANG=55 deg in COMMON section.	#2
12787.002	FLAG	Delete FLAG=1 in COMMON section, but add "Not possible to assign to 82Se" under COMMENT.	This comment was the definition of FLAG=1 but deleted in TRANS.1336.
12989.003	POL-BM	Delete POL-BM=0.60 in DATA section.	#3
13126.002	E-LVL	Delete E-LVL=3.74 MeV in DATA section.	#3

13913.002	ERR-T	Delete ERR-T=0.17 in DATA section.	#1 (single data point dataset)
13913.003	ERR-T	Delete ERR-T=0.012 in DATA section.	#1 (single data point dataset)
13923.003	E-ERR	Delete E-ERR-1 keV in COMMON but add "~+/-1 keV overall energy scale uncertainty is not included" under ERR-ANALYS.	See p.240.
14125.019	EN	Delete EN=4.1 MeV in COMMON section.	#2
14125.019	EN-ERR	Delete EN-ERR=0.1 MeV in COMMON section.	#2
14654.002	DECAY-FLAG	Delete DECAY-FLAG=1 in COMMON section. Also delete (1.) under DECAY-DATA.	Decay data of REACTION denominator
20070.002	E-LVL	Delete E-LVL=0 MeV in COMMON section.	#2
20338.013	ERR-T	Delete ERR-T=25.4% in COMMON section.	#1 Value in error table
20394.003	ERR-T	Delete ERR-T=4.21% in COMMON section.	#1 Value in error table
20828.003	MOMENTUM L	Delete MOMENTUM L=0.0 in COMMON section.	#2
20828.003	SPIN J	Delete SPIN J=0.5 in COMMON section.	#2
21102.049	ANG	Delete ANG=15 deg in COMMON section.	#3
21102.049	ANG-RSL	Delete ANG-RSL=15 deg in COMMON section.	#3
21494.002	ERR-T	Delete ERR-T=1.8% in COMMON section.	#1
21494.009	ERR-T	Delete ERR-T=2.8% in COMMON section.	#1
21698.005	ERR-2	Delete ERR-2 in DATA section?	Calculated by the compiler in 1980s? The entry in 1980s mentions "These two contributions are added in quadrature and given in the data table".
21808.020	MISC1-ERR	MISC1-ERR -> MISC2-ERR, MISC2-ERR -> MISC3	
21808.021	MISC1-ERR	DATA(-ERR) -. MISC1(-ERR), MISC1 -> MISC2, MISC1-ERR (in COMMON section) -> MISC2-ERR, MISC1-ERR (in DATA section) -> MISC3, MISC2-ERR -> MISC3-ERR, MISC2 -> DATA, MISC3 -> DATA-ERR	
21965.004	ERR-12	Delete ERR-12=0.2% in COMMON section.	Value in error table
22307.002	ERR-T	Delete ERR-T=0.46 b in DATA section.	
22340.004	ERR-1	Delete ERR-1=4.20% in COMMON section.	Wrongly copied from 009?

22340.008	ERR-1	Delete ERR-1=4.20% in COMMON section.	Wrongly copied from 009?
22499.033	EN-MEAN	Delete EN-MEAN=75 keV in DATA section.	#3
22801.005	MONIT-ERR	Delete MONIT-ERR in DATA section.	#1 (MONIT-ERR/MONIT in DATA section is 1.5%)
22801.006	MONIT-ERR	Delete MONIT-ERR in DATA section.	#1 (MONIT-ERR/MONIT=1.5% in DATA section.)
22871.002	MONIT-ERR	Delete MONIT-ERR=0.1 b in DATA section.	#1 (MONIT-ERR/MONIT=0.75% in DATA section.)
22921.005	ERR-SYS	Delete ERR-SYS in DATA section.	#1 (ERR-SYS/DATA=2% in DATA section.)
22953.003	ERR-T	Delete ERR-T in DATA section.	#1 (ERR-T/DATA=5% in DATA section.)
22964.002	ERR-T	Delete ERR-T in COMMON section. ERR-T -> DATA-ERR in DATA section?	3.09% does not include contribution from monitor reaction. I do not understand why the quadrature sum of the total uncertainties in Table 2 (4.2%) does not agree with the uncertainty in Table 4 (7.9/204.8=3.9%).
22964.002	MONIT-ERR	Delete MONIT-ERR=2.89% in COMMON section and MONIT-ERR=0.1 b in DATA section, but ERR-14 -> MONIT-ERR	MONIT-ERR/MONIT=0.75% in Data section
22964.003	ERR-T	ERR-T -> DATA-ERR in DATA section?	The total uncertainty is 7.42% in Table 3 but 214/3038=7.04% in Table 4.
22964.003	MONIT-ERR	Delete MONIT-ERR=0.3 b in DATA section.	MONIT-ERR/MONIT=2.14% in DATA section is different from 3.13% in RI.

22993.002	ERR-T	Move ERR-S=1% and ERR-T=4% in free text?	Typical uncertainty values coded in COMMON?
23427.004	TEMP	Delete TEMP=180 deg-C in DATA section.	#3
23427.005	TEMP	Delete TEMP=180 deg-C in DATA section.	#3
23439.002	E-LVL	Delete E-LVL=2.9 MeV in COMMON section. Swap E-LVL and E-EXC-MEAN in DATA section (recom.)	#2
23515.002	ERR-T	Delete ERR-T=0.03 b.	#1
30777.003	DATA-ERR	(Recompiled at NDS)	
30833.003	ASSUM1-ERR	Delete ASSUM1-ERR=0.09 b in DATA section.	#1
30833.003	ASSUM2-ERR	Delete ASSUM2-ERR=28 b in DATA section.	#1
30833.003	ASSUM3-ERR	Delete ASSUM3-ERR=0.35 b in DATA section.	#1
30843.003	ASSUM1-ERR	Delete ASSUM1-ERR=0.09 b in DATA section.	#1
30843.003	ASSUM2-ERR	Delete ASSUM2-ERR=28 b in DATA section.	#1
30843.003	ASSUM3-ERR	Delete ASSUM3-ERR=8 b in DATA section.	#1
30999.003	EN-ERR	Delete EN-ERR=0.23 MeV in COMMON section (Energy uncertainty of the monitor cross section.)	Another solution is to replace EN-ERR with EN-NRM-ERR though the heading is undefined.
30999.004	EN-ERR	Delete EN-ERR=0.23 MeV in COMMON section (Energy uncertainty of the monitor cross section.)	Another solution is to replace EN-ERR with EN-NRM-ERR though the heading is undefined.
31401.003	EN-ERR	Delete EN-ERR=0.40 MeV in COMMON section (Energy uncertainty of the monitor cross section.)	Another solution is to replace EN-ERR with EN-NRM-ERR though the heading is undefined.
31687.002	ANG	ANG -> ANG-ERR in COMMON section. Explain it as "Systematic error in angle determination".	c.f. p.183 "one tenth of a degree".
40112.010	EN	Delete EN=2.5300E-02 eV in COMMON section.	#2
40238.007	ANG-CM	Delete ANG-CM=61 deg in COMMON section.	#2
40324.014	ANG	Delete ANG=61 deg in COMMON section.	#2

40324.018	ANG	Delete ANG=91 deg in COMMON section.	#2
40552.003	ERR-T	Delete ERR-T=0.047 b in COMMON section.	#1 (single data point dataset)
40553.003	ERR-T	Delete ERR-T=23 mb in COMMON section.	#1 (single data point dataset)
40636.002	MONIT	EN-NRM -> EN-NRM1, MONIT -> MONIT1 in COMMON section, add EN-NRM2=2.5 MeV, MONIT -> MONIT2 in DATA section. Explain two normalization methods in free text.	
40636.004	MONIT	EN-NRM -> EN-NRM1, MONIT -> MONIT1 in COMMON section, add EN-NRM2=2.5 MeV, MONIT -> MONIT2 in DATA section. Explain two normalization methods in free text.	
40636.006	MONIT	EN-NRM -> EN-NRM1, MONIT -> MONIT1 in COMMON section, add EN-NRM2=2.5 MeV, MONIT -> MONIT2 in DATA section. Explain two normalization methods in free text.	
40636.008	MONIT	EN-NRM -> EN-NRM1, MONIT -> MONIT1 in COMMON section, add EN-NRM2=2.5 MeV, MONIT -> MONIT2 in DATA section. Explain two normalization methods in free text.	
40980.010	EN	Delete EN=145 keV in COMMON section.	#2
41124.003	STAT-W G	Delete STAT-W G=0.5 in COMMON section.	#2
41451.002	E-ERR	E-ERR -> E-DN-ERR (in COMMON section) or E-NM-ERR (in DATA section)	
A0480.040	EN	Delete EN=22.6 MeV in COMMON section.	#2
A0937.002	ANG	Delete ANG=0 deg in COMMON section.	
A1432.007	E-LVL	Delete E-LVL=0 MeV in COMMON section.	#2
A1501.002	E-LVL	Delete E-LVL=0 MeV in COMMON section.	#2
A1527.006	E-LVL	Delete E-LVL=0 MeV in COMMON section. Fig.12 -> Figs.12-13 in STATUS.	#2
A1527.007	E-LVL	Delete E-LVL=0 MeV in DATA section.	#3
C0132.007	DATA-ERR	Move DATA-ERR=12% in COMMON section to C0132.001 with DATA-ERR -> ERR-1	
C0132.008	DATA-ERR	Move DATA-ERR=12% in COMMON section to C0132.001 with DATA-ERR -> ERR-1	
C0132.009	DATA-ERR	Move DATA-ERR=12% in COMMON section to C0132.001 with DATA-ERR -> ERR-1	
C0132.010	DATA-ERR	Move DATA-ERR=12% in COMMON section to C0132.001 with DATA-ERR -> ERR-1	
C0132.011	DATA-ERR	Move DATA-ERR=12% in COMMON section to C0132.001 with DATA-ERR -> ERR-1	
C0405.008	EN-MAX	Delete EN-MAX=80 keV in COMMON section.	
C0405.008	EN-MIN	Delete EN-MIN=0 keV in COMMON section.	
C0499.002	EN-ERR	EN-ERR in COMMON section -> EN-ERR1 (uncertainty at gas cell entrance) and EN-ERR in DATA section -> EN-ERR2 (uncertainty at gas cell exit)	

C0595.012	DATA-ERR	Delete DATA-ERR=5% in DATA section (c.f. HISTORY).	
C0731.004	DATA-ERR	Delete DATA-ERR=10% in COMMON section.	#2. The letter from Norman does not provide the cross section uncertainty at the high energy region.
C0925.062	ERR-S	Delete ERR-S=1.0 mb in COMMON section.	#3
C1103.002	DATA-ERR	DATA-ERR -> ERR-1 (scale uncertainty) in COMMON section.	
C1111.002	DATA-ERR	DATA-ERR -> ERR-SYS (absolute uncertainty) in COMMON section.	
C1111.003	DATA-ERR	DATA-ERR -> ERR-SYS (absolute uncertainty) in COMMON section.	
C1571.003	EN-ERR	E-EXC -> E-EXC-CMP and EN-ERR -> E-EXC-C-ER in DATA section.	
C1832.008	ANG	Delete ANG=90 deg in COMMON section.	#2
C1832.009	ANG	Delete ANG=90 deg in COMMON section.	#2
C1918.004.1	ERR-T	Delete ERR-T=3 keV in COMMON section.	c.f. p.474
C2068.008	PARITY	Delete PARITY=-1.0 in COMMON section. (J of residual 19F)	c.f. p.1227 (right)
C2068.008	SPIN J	Delete SPIN J=0.5 in COMMON section. (J of residual 19F)	c.f. p.1227 (right)
C2068.009	PARITY	Delete PARITY=-1.0 in COMMON section. (J of residual 19F)	c.f. p.1227 (right)
C2068.009	SPIN J	Delete SPIN J=0.5 in COMMON section. (J of residual 19F)	c.f. p.1227 (right)
C2068.010	PARITY	Delete PARITY=1.0 in COMMON section. (J of residual 19F)	c.f. p.1227 (right)
C2068.010	SPIN J	Delete SPIN J=2.5 in COMMON section. (J of residual 19F)	c.f. p.1227 (right)
C2068.011	PARITY	Delete PARITY=1.0 in COMMON section. (J of residual 19F)	c.f. p.1227 (right)
C2068.011	SPIN J	Delete SPIN J=2.5 in COMMON section. (J of residual 19F)	c.f. p.1227 (right)
C2303.002	DATA-ERR	DATA-ERR -> ERR-SYS in COMMON and treat it as the upper limit (absolute scale).	
C2335.003	EN	Delete EN=27.0 MeV in COMMON. Fig. 4 -> Fig. 2 in STATUS.	Elab=27 MeV for Fig.4.
D0034.002	DATA-ERR	DATA-ERR -> ERR-1 in COMMON section and ERR-ANALYS.	
D0295.002	DATA-ERR1	Delete DATA-ERR1=3% in COMMON section and DATA-ERR1 -> DATA-ERR (Free text may be kept.)	
D0295.004	DATA-ERR1	Delete DATA-ERR1=3% in COMMON section and DATA-ERR1 -> DATA-ERR (Free text may be kept.)	
D0295.006	DATA-ERR1	Delete DATA-ERR1=3% in COMMON section and DATA-ERR1 -> DATA-ERR (Free text may be kept.)	
D0295.010	DATA-ERR1	Delete DATA-ERR1=3% in COMMON section and DATA-ERR1 -> DATA-ERR (Free text may be kept.)	

D0295.012	DATA-ERR1	Delete DATA-ERR1=3% in COMMON section and DATA-ERR1 -> DATA-ERR (Free text may be kept.)	
D0574.002	EN-ERR	Delete EN-ERR=0.2 MeV in COMMON section.	I do not know where the compiler found this value.
D4312.004	EN-ERR	EN-ERR -> EN-RSL-HW in DATA section (energy step of thick target yield measurement)	
D4312.005	EN-ERR	EN-ERR -> EN-RSL-HW in DATA section (energy step of thick target yield measurement)	
D4380.002	ANG	Delete ANG=16 deg in COMMON section.	#2
D5176.002	E-LVL	Delete E-LVL=0.0 MeV in COMMON section.	#2
D6016.002	EN	Delete EN=95.0 MeV in COMMON section.	95 MeV is one of the initial proton beam energies
D6016.003	EN	Delete EN=95.0 MeV in COMMON section.	95 MeV is one of the initial proton beam energies
D6016.004	EN	Delete EN=95.0 MeV in COMMON section.	95 MeV is one of the initial proton beam energies
D6016.005	EN	Delete EN=95.0 MeV in COMMON section.	95 MeV is one of the initial proton beam energies
D6016.006	EN	Delete EN=95.0 MeV in COMMON section.	95 MeV is one of the initial proton beam energies
D6016.007	EN	Delete EN=95.0 MeV in COMMON section.	95 MeV is one of the initial proton beam energies
D6016.008	EN	Delete EN=95.0 MeV in COMMON section.	95 MeV is one of the initial proton beam energies
D6016.009	EN	Delete EN=95.0 MeV in COMMON section.	95 MeV is one of the initial proton beam energies
D6016.010	EN	Delete EN=95.0 MeV in COMMON section.	95 MeV is one of the initial proton beam energies
D6016.011	EN	Delete EN=95.0 MeV in COMMON section.	95 MeV is one of the initial proton beam energies
E1748.039	ANG1	Delete ANG-1=30 deg in COMMON section.	#2
E1748.039	ANG2	Delete ANG-2=30 deg in COMMON section.	#2
F0110.002	EN	Delete EN=7.0 MeV in COMMON section.	#2
F0239.019	E	E=124 keV+124 keV+129 keV must be E=124 keV+125 keV+129 MeV.	c.f. Table 3
F0811.003	EN	Delete EN=40 MeV in COMMON section.	#2

F1191.009	DATA-ERR	DATA-ERR -> ERR-DIG in COMMON section?	
F1191.010	DATA-ERR	DATA-ERR -> ERR-DIG in COMMON section?	
F1191.011	DATA-ERR	DATA-ERR -> ERR-DIG in COMMON section?	
F1422.003	EN	EN -> E	
F1422.003	EN-ERR	EN-ERR -> E-ERR	
L0241.003	ERR-S	Delete ERR-S=0.7% in COMMON section (could be a part of free text under ERR-ANALYS).	c.f. Table IV
M0082.002	EN-MAX	Delete EN-MAX=20 MeV in COMMON section.	#2
M0450.005	DATA-ERR	Delete DATA-ERR=0.003 mb*MeV in DATA section (c.f. 006)	#1
M0580.002	ANG	Delete ANG=135 deg in COMMON section.	#2
M0595.002	ANG	Delete ANG=45 deg in COMMON section.	#2
M0852.002	ERR-T	Delete ERR-T=10% in COMMON section.	#1
M0852.003	ERR-T	Delete ERR-T=9.5% in COMMON section.	#1
M0873.009	EN-MAX	Delete EN-MAX=200 MeV in COMMON section.	#2
M0873.009	EN-MIN	Delete EN-MIN=150 MeV in COMMON section.	#2
M0935.002	ERR-T	Delete ERR-T=12.0% in COMMON section.	#1
M0935.003	ERR-T	Delete ERR-T=12.0% in COMMON section.	#1
M0935.004	ERR-T	Delete ERR-T=9.0% in COMMON section.	#1
M1003.003	EN-MAX	Delete EN-MAX=82.0 MeV in COMMON section.	#2
O0331.004	ERR-DIG	Delete ERR-DIG=0.006 mb/sr in COMMON section.	#2
O0777.002	ERR-2	Delete ERR-2=13% in COMMON section.	#2
O0863.024	E	Delete E=1173 keV in COMMON section.	#2
O0863.026	E	Delete E=932 keV in COMMON section.	#2
O0865.002	ERR-S	Delete ERR-S=5% in COMMON section. Replace ERR-S values in the DATA section with those digitized from Fig.2.	#1
O0951.002	ERR-T	Delete ERR-T=5% in COMMON section. (5% is the upper limit.)	#1
O1033.004	DATA-ERR	Delete DATA-ERR=10% in COMMON section. (10% is the upper limit.)	#1
O1567.013	ANG-ERR	ANG-ERR -> ANG-ERR-D in COMMON section?	
O2476.002	ERR-S	Delete ERR-S=1.0% in COMMON section.	#1

T0276.007	EN-ERR	Delete EN-ERR=0.3% to COMMON section? (Energy error in the initial beam energy.)	Another solution could be to replace EN-ERR with EN-RSL. (The supplemental material compiling the data PAPS PRVCA-20-88-4 is not available at NDS.)
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