

ENSDF Nuclear Data Evaluation Instructions

⚠ CRITICAL WORKFLOW REMINDER ⚠

ALWAYS START WITH: `git status`

- Before any "What changed?" workflow
- Before any change detection or documentation
- This ensures ALL modified files are identified and processed
- Missing this step = incomplete change tracking!

CRITICAL FORMATTING RULE: ALL ENSDF values AND uncertainties MUST be LEFT-JUSTIFIED in their fields!

- Energy values, RI values, half-lives, $J-\pi$, AND their uncertainties (DE, DRI, DT, etc.)
- Special markers (GT, LT) within uncertainty fields are also left-justified
- NEVER right-justify or center ANY ENSDF field content!

Command Triggers

"Self-Calibrate Columns"

Execute column validation on current ENSDF file:

- **PowerShell:** `.\column-calibrate.ps1 "currentfile.ens"` (add `-Detailed` for character mapping)
- **Python:** `python column_calibrate.py "currentfile.ens"` (add `--detailed` for character mapping)

Process: Display 80-char ruler → Extract L/G records → Validate against ENSDF Manual → Report issues

"What changed?"

MANDATORY FIRST STEP: Always run `git status` to identify ALL modified files.

Execute comprehensive change detection and documentation:

1. **FIRST:** Run `git status` to list all modified files
2. **For each file:** Run `git diff HEAD~1 "filename"` to see what changed
3. Update `change.log` with evidence-based entries (never assume changes)
4. Document with line numbers, before/after content, and scientific/technical context

Remember: Git status MUST be the first step - missing files means incomplete documentation! Use git diff to see specific changes in each file.

"Fix format!"

Auto-convert text to proper ENSDF notation:

- Greek letters: `35S` → `{+35}S`, α → `|a`, β → `|b`, etc.
- Math symbols: \times → `|*`, \approx → `|?`, \pm → `|+`, etc.
- Superscripts/subscripts: Use `{+n}` and `{-n}` format

ENSDF Column Format Standards (CRITICAL - NO MISTAKES ALLOWED)

L-Record Format (Energy Levels):

Columns:
12345678901234567890123456789012345678901234567890123456789012345678901234567890
Format: 35XX L EEEE.E DE JP T DT L S
DS C
Example: 35P L 1572.0 1 1/2+ 2.29 PS 14 2 1.23
45

Field	Columns	Required	Description
NUCID	1-5	✓	Nucleus (e.g., "35P ")
CONT	6		Continuation flag
BLANK	7	✓	Must be blank
TYPE	8	✓	"L"
BLANK	9	✓	Must be blank
E	10-19	✓	Level energy (LEFT-JUSTIFIED)
DE	20-21		Energy uncertainty (LEFT-JUSTIFIED)
SPACE	22	✓	Readability space
J	23-39		Spin-parity (LEFT-JUSTIFIED at col 23)
T	40-49		Half-life with units (LEFT-JUSTIFIED)
DT	50-55		Half-life uncertainty (LEFT-JUSTIFIED)
L	56-64		Angular momentum transfer
S	65-74		Spectroscopic strength
DS	75-76		Uncertainty in S (LEFT-JUSTIFIED)
C	77		Comment flag

G-Record Format (Gamma Transitions):

Columns:
12345678901234567890123456789012345678901234567890123456789012345678901234567890
Format: 35XX G EEEE.E DE II.I DI [M] MR DMR CC DCC TI
DTI C
Example: 35P G 1572.0 1 100.0 4 [E2] 1.23 0.45 0.0368 8 1.23
45

Field	Columns	Required	Description
NUCID	1-5	✓	Nucleus (e.g., "35P ")
CONT	6		Continuation flag
BLANK	7	✓	Must be blank
TYPE	8	✓	"G"
BLANK	9	✓	Must be blank
E	10-19	✓	Gamma energy (LEFT-JUSTIFIED)
DE	20-21		Energy uncertainty (LEFT-JUSTIFIED)
SPACE	22	✓	Readability space
RI	23-29		Relative photon intensity (LEFT-JUSTIFIED at col 23)
DRI	30-31		Uncertainty in RI (LEFT-JUSTIFIED, including GT, LT markers)
M	32-41		Multipolarity
MR	42-49		Mixing ratio
DMR	50-55		Uncertainty in MR (LEFT-JUSTIFIED)
CC	56-62		Conversion coefficient
DCC	63-64		Uncertainty in CC (LEFT-JUSTIFIED)
TI	65-74		Total transition intensity
DTI	75-76		Uncertainty in TI (LEFT-JUSTIFIED)
C	77		Comment flag

Critical: ENSDF files are parsed by automated systems requiring exact positions. One column off = data rejection.

UNCERTAINTY LEFT-JUSTIFICATION RULE: ALL uncertainties (DE, DRI, DMR, DCC, DTI, DT, DS, etc.) MUST be left-justified in their respective fields, just like the values themselves. Special markers (GT, LT) within uncertainty fields are also left-justified.

LEFT-JUSTIFICATION RULE: ALL values AND uncertainties MUST be left-justified within their respective fields. This includes:

- Energy values (E field) and their uncertainties (DE field)
- $J-\pi$ values (spin-parity) and any associated uncertainties
- Half-life values (T field) and their uncertainties (DT field)
- RI values (relative intensity) and their uncertainties (DRI field)
- Mixing ratios (MR field) and their uncertainties (DMR field)
- Conversion coefficients (CC field) and their uncertainties (DCC field)
- All numerical and text values AND their uncertainties Never right-justify or center ANY values OR uncertainties in ENSDF records!

Essential Rules

File Protection

- **NEVER** edit `.old` files (reference files from previous evaluation rounds)
- **NEVER** modify first/last line indentation or spacing in `.ens` files
- **ALWAYS** preserve "PN" line with its numeric value
- Make all edits between first and last line boundaries only

Column Positioning

- **J- π placement:** Always start at column 23, LEFT-JUSTIFIED (never add spaces that shift uncertainties)
- **Energy values:** LEFT-JUSTIFIED in their designated columns (10-19)
- **RI values:** Start at column 23, **LEFT-JUSTIFIED** in 7-char field (23-29)
- **DRI values:** Position at columns 30-31 (including special markers like GT, LT)
- **Half-life values:** LEFT-JUSTIFIED in T field (columns 40-49)
- **BR values:** Position at column 32 (N-records), LEFT-JUSTIFIED
- **NR values:** Columns 11-15 (N-records), LEFT-JUSTIFIED

CRITICAL: ALL values must be LEFT-JUSTIFIED within their respective fields - never right-justified or centered!

⚠ CRITICAL COLUMN RULE: When fixing a quantity's position to the correct columns, NEVER shift other field values to wrong columns!

- L-transfer values: Must stay in columns 56-64
- Spectroscopic factors: Must stay in columns 65-74
- Comment flags: Must stay in column 77
- Only adjust spacing between fields - never move field data to incorrect columns!

NSR Keynumber Formatting

- **In comments/records:** Second letter lowercase (`2023Bo17`, `2021Wa16`)
- **In headers/Q-records:** All uppercase (`2023B017`, `2021WA16`)

Change Tracking

- **Always** update `.vscode/change.log` after significant changes
- **Never** create duplicate `change.log` files
- Use evidence-based documentation with specific line numbers
- **Never** document assumed changes - always verify with tools

ENSDF Special Characters

Superscripts/Subscripts

- `{+n}` → superscript (e.g., `{+35}Ar` → ^{35}Ar)
- `{-n}` → subscript (e.g., `T{-1/2}` → $T_{1/2}$)
- `{+-n}` → negative superscript (e.g., `{+-4}` → $^{-4}$)

Greek Letters

Lowercase: |a → α, |b → β, |g → γ, |d → δ, |e → ε, |l → λ, |m → μ, |n → ν, |p → π, |r → ρ, |s → σ, |t → τ, |w → ω **Uppercase:** |D → Δ, |G → Γ, |L → Λ, |P → Π, |S → Σ, |W → Ω

Mathematical Symbols

- |* → × (times), |? → ≈ (approx), |+ → ± (plus-minus), |- → ∓ (minus-plus)
- |< → ≤, |> → ≥, |' → °, |= → ≠, |@ → ∞
- |^ → ↑, |_ → ↓, |(→ ←, |) → →, |. → α, || → |

Important: Use |? for approximate values, never standalone ~ (except in names/mass notation)

Common Examples

- |(e+|b{++})p → %(ε+β⁺)p
- {+208}Pb({+36}S,{+35}S) → ²⁰⁸Pb(³⁶S,³⁵S)
- |s(E({+3}He),|q) → σ(E(³He),θ)

Academic Standards

Citation Tense

Use PAST tense for all references to completed studies:

- ✓ "Authors stated...", "1994FO04 measured...", "Previous evaluators concluded..."
- X "Authors state...", "1994FO04 measures..."

Grammar Fixes

Common corrections: "stoped" → "stopped", "usign" → "using", "coefficients" → "coefficients"

Nuclear Data Evaluation

General Comment Ordering (adopted.ens files)

1. **Isotope discovery** (reference): experimental details
2. **{+A}X production**: production methods and studies
3. **{+A}X decay measurements**: half-life, decay modes
4. **{+A}X radius measurement**: nuclear radius determinations
5. **{+A}X mass measurements**: mass spectrometry, Q-values
6. **Theoretical calculations**: models, predictions (always last)

L-Transfer Rules for J-π Assignment

- L=0 → J-π: 1/2+
- L=1 → J-π: 1/2-, 3/2-
- L=2 → J-π: 3/2+, 5/2+
- L=3 → J-π: 5/2-, 7/2-

Note: Always confirm with experimental data; never enter L-values in J-π column.

Tools and Workflows

PDF Generation

```
# Single element
Set-Location "D:\X\ND\Files"
$element = "Al"
Get-ChildItem "D:\X\ND\A35\finished\${element}35\new\*.ens" | ForEach-Object {
    java -jar "D:\X\ND\McMaster-MSU-Java-
NDS\McMaster_MSU_JAVA_NDS_v3.0_01May2025.jar" $_.FullName "${($_.BaseName)}.pdf"
}

# All elements
$elements = @("Al", "Ar", "Ca", "K", "Mg", "Na", "Ne", "P", "Si")
foreach ($element in $elements) {
    Get-ChildItem "D:\X\ND\A35\finished\${element}35\new\*adopted.ens" | ForEach-
Object {
        java -jar "D:\X\ND\McMaster-MSU-Java-
NDS\McMaster_MSU_JAVA_NDS_v3.0_01May2025.jar" $_.FullName "${($_.BaseName)}.pdf"
    }
}
```

Change Detection Process

1. **Pre-work (MANDATORY):** `git status`, `git diff --name-only HEAD`
2. **During work:** Track file modifications systematically
3. **Post-work:** Use all detection tools on ALL files from `git status`
4. **Documentation:** Evidence-based `change.log` entries with line numbers

CRITICAL REMINDER: Always start with `git status` - this shows the complete picture!

File Categories to Track

- **ENSDF source files:** *.ens files (most important)
- **Generated PDFs:** *.pdf files (expected to change when source changes)
- **Processing artifacts:** temp/. files (expected, document but don't commit)
- **Tools and scripts:** .vscode/. files (important for tooling changes)
- **Documentation:** README.md, change.log, etc.

Evidence-Based Documentation Rules

Every change log entry should be backed by:

- Specific file diffs from `git diff HEAD~1 "filename"`
- Line numbers where changes occurred
- Actual before/after content when significant
- Explanation of why the change was made

Key principle: Use multiple detection methods and always cross-verify. If `git` shows a file changed, dig deeper with `git diff`. If you modified an ENSDF file, expect to see corresponding PDF changes.

Verification Checklist

- ☐ **FIRST:** `git status` - identify ALL modified files (MANDATORY)
- ☐ `git diff --name-only HEAD` - complete list verification
- ☐ `git ls-files --others --exclude-standard` - untracked files
- ☐ `git diff HEAD~1 "filename"` on each modified file from git status
- ☐ Update `change.log` with evidence-based entries
- ☐ Comprehensive commit message
- ☐ Cross-check: did any ENSDF changes result in expected PDF updates?

Remember: Start every workflow with git status!

Git Commit Template

Title: Brief description of main changes

Summary:

- Enhanced/improved/fixed major components
- Scientific content updates in specific files

ENSDF Tools:

- `tool_name.py`: Specific improvements and validation results

Scientific Content:

- `file_name.ens`: Changes with line numbers and rationale

Processing Artifacts:

- PDF files: Regenerated files listed
- Temp files: Expected analysis output updates

Files changed: X modified, Y untracked

Brief scope and impact summary

Example Commit Structure

Title: Enhance ENSDF column calibration tools and improve Ar35 scientific content

Summary:

- Enhanced Python column calibration script with complete 80-column ENSDF format support
- Improved scientific content and formatting in Ar35 ENSDF files
- Completed comprehensive change tracking and documentation

ENSDF Tools:

- `column_calibrate.py`: Extended from 41-column to complete 80-column ENSDF support
- `check_averages.py`: Completed and tested average calculation verification tool

Scientific Content:

- `Ar35_36ar_p_d.ens`: Fixed grammar in L=3 vs L=2 comparison (line 77)
- `Ar35_adopted.ens`: Multiple scientific and formatting enhancements

Processing Artifacts:

- PDF files: Regenerated Ar35_36ar_3he_a.pdf, Ar35_36ar_p_d.pdf, Ar35_adopted.pdf
- Temp files: Updated all analysis outputs (35.err, 35.fed, 35.fmt, etc.)

Files changed: 15 modified, 2 untracked

Completion of comprehensive ENSDF column calibration tooling and systematic improvement of Ar35 nuclear data content.

Project Structure

Core Files (Most Critical)

- `finished/[Element]/new/*.ens` - Primary ENSDF source files
- `.vscode/change.log` - Comprehensive change tracking

Generated Files (Expected to Change)

- `finished/[Element]/pdf/*.pdf` - Generated from .ens files
- `finished/[Element]/temp/*.*` - Analysis tool artifacts

Tools

- `ens2pdf.py` - Python script for automated ENSDF to PDF conversion
- `.vscode/column-calibrate.ps1` - PowerShell column validator
- `.vscode/column_calibrate.py` - Python column validator
- `.vscode/check_averages.py` - Average calculation validator

Reference Files (NEVER EDIT)

- `*.old` files - Previous evaluation rounds, keep untouched

Focus Areas

Current Priority: K35 and P35 files (Ar35 completed)

Quality Assurance: Use Self-Calibrate Columns before any ENSDF edits, use What changed? after any modifications

Remember: Nuclear data accuracy is critical - when in doubt, verify with tools and cross-check against ENSDF Manual specifications.