Preparation of the IDB Spectra

1. Overview

The spectral information and associated metadata, including source information, detector setup, and shielding configuration is described in human readable, comma-separated text files (csv). Six csv files are associated with each material type and include the following information (where [*Isotope*] is U, Pu, and MOX):

[*Isotope*]_measurement_metadata
Metadata of the measurement configuration, including material composition at time of acquisition (decay corrected from certificate date). Data that is unique to a measurement configuration e.g. detector geometry, source-detector distance, analyzer and other electronics used, attenuating materials are provided in this file.

[*Isotope*]_spectrum_metadata
The information that is unique to the spectrum. This includes detector specifications (e.g. date of acquisition, number of channels, gain (keV/channel), energy range, real and live time, full width half-maximum (FWHM) of the 186 or 208 peak for uranium or plutonium measurements, respectively.

[*Isotope*]_source_metadata
The source material used for the measurement, this includes the ratio and uncertainties of isotopes present and processing information of the material. In addition, the certificate information for the source material is listed.

[*Isotope*]_spectrum_counts_metadata
The counts per channel for each spectrum. This data is linked via the UID.spectrum index to the measurement_metadata file.

[*Isotope*]_spectrum_checksum_metadata
The MD5 checksum for the original spectrum file. This data is linked via the UID.spectrum index to the measurement_metadata file. This information is provided to prevent duplication of entries in the database.

[*Isotope*]_provenance
Details on the csv data provider, including laboratory and contract information.

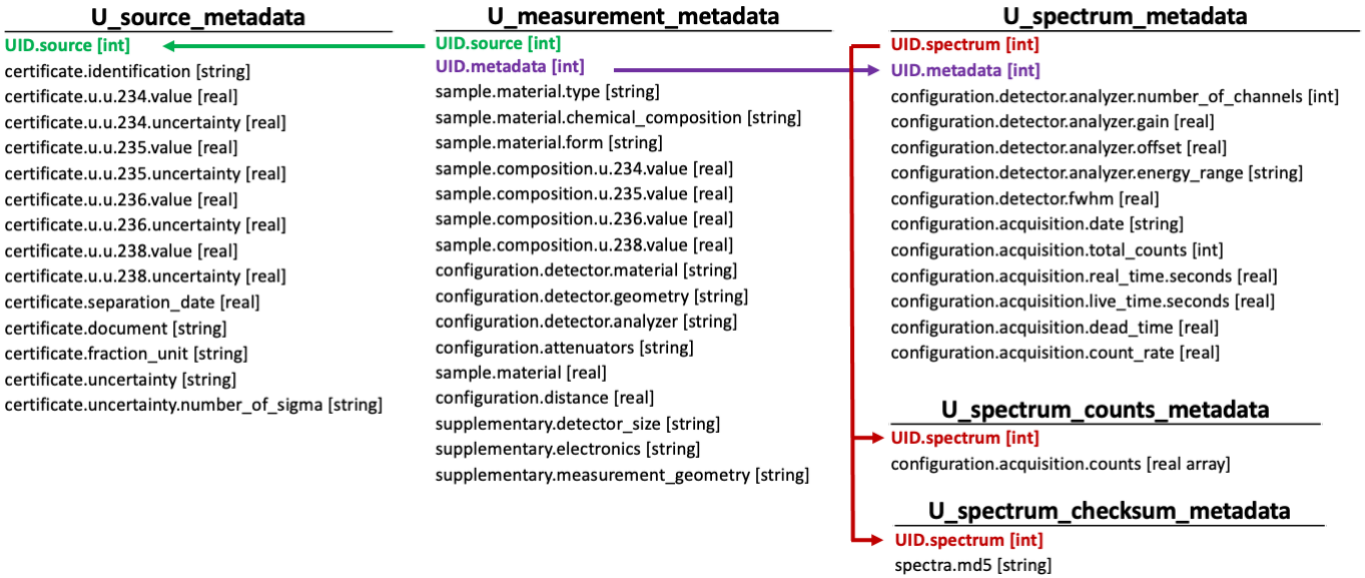

Figure 1 Schema of the five csv files for spectra taken of uranium bearing materials. The five files are linked by integer values UID.source, UID.metadata, and UID.spectrum.

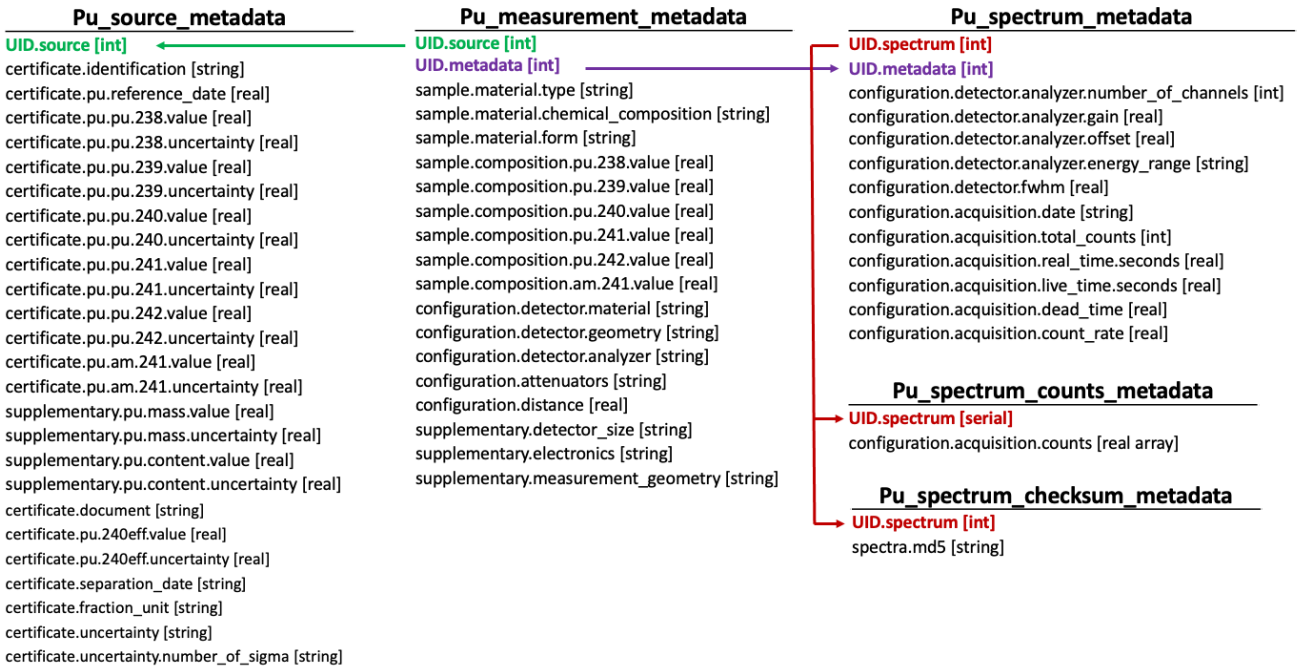

Figure 2 Schema of the five csv files for spectra taken of plutonium bearing materials. The five files are linked by integer values UID.source, UID.metadata, and UID.spectrum.

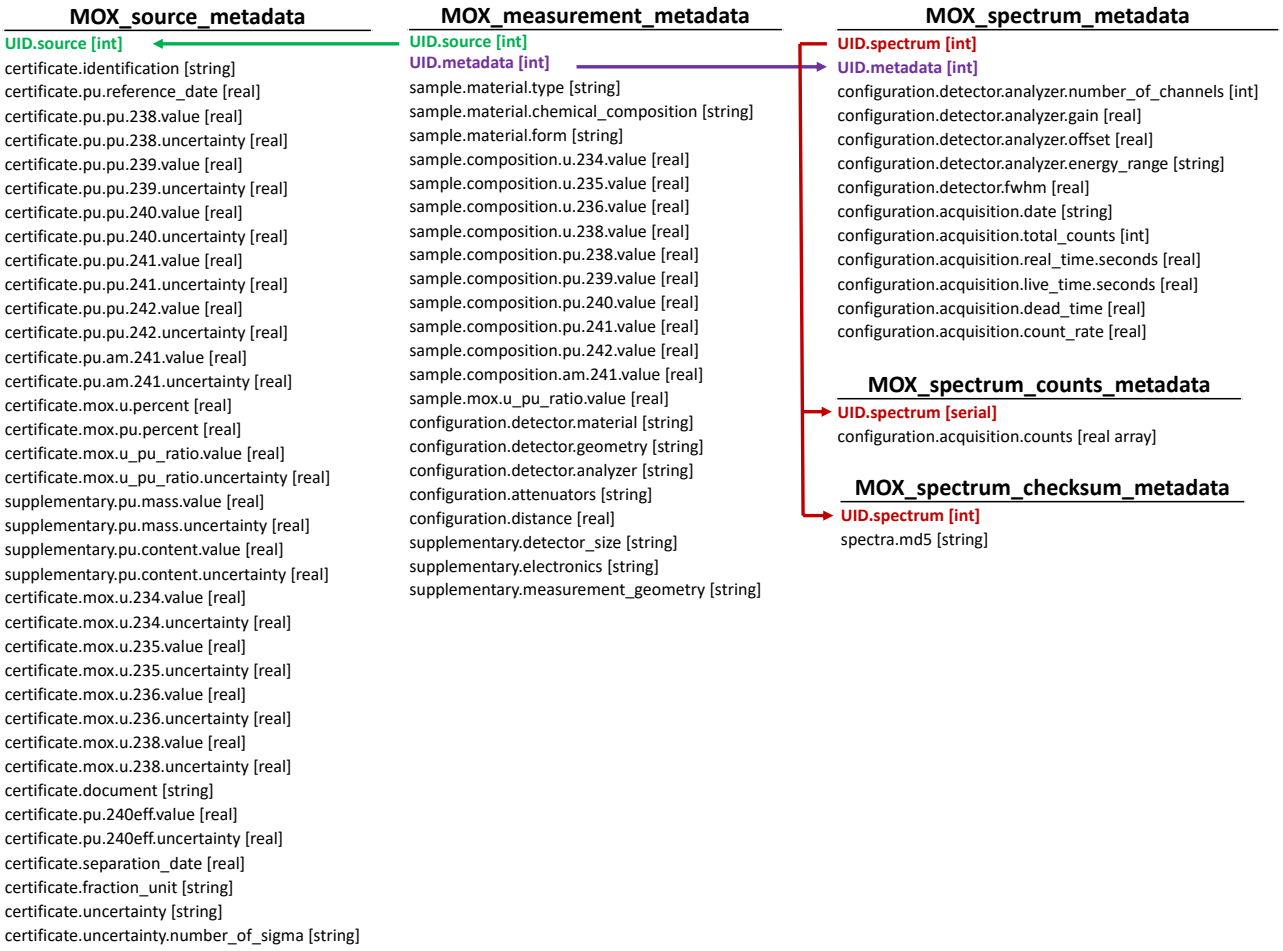

Figure 3 Schema of the five csv files for spectra taken of MOX bearing materials. The five files are linked by integer values UID.source, UID.metadata, and UID.spectrum.

2. Preparation of "IRDB_reference_spectra.xls"

The entries in each csv metadata file and corresponding entry in the IRDB_reference_spectra.xls Excel file are listed below.

Uranium

U_measurement_metadata	Reference in IRDB_reference_spectra.xls	Data type and Format	Description
UID.metadata	Unique ID		
UID.source	Unique ID to U_source_metadata		
sample.material.type	Read from spectrum file path	String	Material measured: U
sample.material.chemical_composition	Column D 'Nature'	String	Chemical compound or physical form of the material: U3O8, UO2, UF6
sample.material.form	Column D 'Nature'	String	Physical form of the material: powder, metal, solution
sample.composition.u.234.value	From certificate	Real	Weight percent (isotopic weight ratio)
sample.composition.u.235.value	From certificate	Real	Weight percent (isotopic weight ratio)
sample.composition.u.236.value	From certificate	Real	Weight percent (isotopic weight ratio)
sample.composition.u.238.value	From certificate	Real	Weight percent (isotopic weight ratio)
configuration.detector.material	Column F 'Detector type'	Real	Detector material: HPGe, NaI, CZT, LaBr3
configuration.detector.geometry	Column F 'Detector type'	Real	Detector geometry: Coax, Planar, Semi-planar
configuration.detector.analyzer	Column G 'Analyser'	String	System analyzer: ORTEC DART, DSPEC, integrated
configuration.attenuators	Column H 'Attenuator (material and thickness in mm)'	String	Attenuator material and the thickness in millimeters. Format Material:Thickness with semicolon delimiter between pairs: Cd:2.0;Pb:1.6
configuration.distance	Column J 'Distance (cm)'	Real	Source to detector distance in centimeters
supplementary.detector_size	Column AJ 'Detector size and/or model'	String	Detector characteristics: 56 mm dia by 56 mm thick coaxial
supplementary.electronics	Column AK 'Acquisition electronics'	String	Measurement electronics: Commercial Analog NIM electronics
supplementary.measurement_geometry	Column AL:AT 'Measurement geometry'	String	Measurement geometry information

U_spectrum_metadata	Reference in IRDB_reference_spectra.xls	Data type and Format	Description
UID.spectrum	Unique ID		
UID.metadata	Unique ID to UID.source		
configuration.detector.analyzer.number_of_channels	Read from spectrum file	Integer	Number of analyzer channels
configuration.detector.analyzer.gain	Read from spectrum file	Real	Gain of analyzer in keV/ch
configuration.detector.analyzer.offset	Read from spectrum file	Real	Offset of analyzer in keV
configuration.detector.analyzer.energy_range	Calculated from spectrum file	String	Energy range of detector in the format "E1-E2 keV"
configuration.detector.fwhm	Calculated from spectrum file	Real	FWHM in keV at 186keV
configuration.acquisition.date	Read from spectrum file	String Date/Time	Date and time spectrum was acquired in UTC
configuration.acquisition.total_counts	Calculated from spectrum file	Integer	Total counts in spectrum
configuration.acquisition.real_time.seconds	Read from spectrum file	Real	Spectrum real time
configuration.acquisition.live_time.seconds	Read from spectrum file	Real	Spectrum live time
configuration.acquisition.dead_time	Read from spectrum file	Real	Spectrum dead time
configuration.acquisition.count_rate	Calculated from spectrum file	Real	Spectrum count rate

U_spectrum_counts_metadata	Reference in IRDB_reference_spectra.xls	Data type and Format	Description
UID.spectrum	Unique ID to U_spectrum_metadata		
configuration.acquisition.counts	Read from spectrum file	String	Comma-separated list of counts per channel, enclosed by brackets

U_spectrum_checksum_metadata	Reference in IRDB_reference_spectra.xls	Data type and Format	Description
UID.spectrum	Unique ID to UID.spectrum		
spectra.md5	Calculated from spectrum file	String, 32 characters	

U_source_metadata	Reference in IRDB_reference_spectra.xls	Data type and Format	Description
UID.source	Unique ID		
certificate.identification	Unique identifier	String	Identifier of certificate: CRM146.NBL0001, CRM146.NBL0002, CRM969.071, CRM969.295, etc.
certificate.u.reference_date	From certificate	String Date/Time	Reference date of certificate in UTC
certificate.u.u.234.value	From certificate	Real	Composition, units given in certificate.fraction_unit
certificate.u.u.234.uncertainty	From certificate	Real	Composition uncertainty
certificate.u.u.235.value	From certificate	Real	Composition, units given in certificate.fraction_unit
certificate.u.u.235.uncertainty	From certificate	Real	Composition uncertainty
certificate.u.u.236.value	From certificate	Real	Composition, units given in certificate.fraction_unit
certificate.u.u.236.uncertainty	From certificate	Real	Composition uncertainty
certificate.u.u.238.value	From certificate	Real	Composition, units given in certificate.fraction_unit
certificate.u.u.238.uncertainty	From certificate	Real	Composition uncertainty
certificate.separation_date	From certificate	String Date/Time	Separation date in UTC
certificate.document	Certificate document name	String	Filename of certificate document, page number: HEU_CRM146.pdf, Page 2
certificate.fraction_unit [string]	From certificate	String	Composition unit weight percent (wt%) or atom percent (at%)
certificate.uncertainty [string]	From certificate	String	Absolute or relative uncertainty
certificate.uncertainty.number_of_sigma [string]	From certificate	String	Number of sigma of uncertainty

Plutonium

Pu_measurement_metadata	Reference in IRDB_reference_spectra.xls	Data type and Format	Description
UID.metadata	Unique ID		
UID.source	Unique ID to Pu_spectrum_checksum_metadata		
sample.material.type	Read from spectrum file path	String	Material measured: Pu
sample.material.chemical_composition	Column Q 'Nature'	String	Chemical compound or physical form of the material: U3O8, UO2, UF6
sample.material.form	Column Q 'Nature'	String	Physical form of the material: powder, metal, solution
sample.composition.pu.238.value	From certificate, decay corrected	Real	Weight percent (isotopic weight ratio)
sample.composition.pu.239.value	From certificate, decay corrected	Real	Weight percent (isotopic weight ratio)
sample.composition.pu.240.value	From certificate, decay corrected	Real	Weight percent (isotopic weight ratio)
sample.composition.pu.241.value	From certificate, decay corrected	Real	Weight percent (isotopic weight ratio)
sample.composition.pu.242.value	From certificate, decay corrected	Real	Weight percent (isotopic weight ratio)
sample.composition.am.241.value	From certificate, decay corrected	Real	Weight percent
configuration.detector.material	Column S 'Detector type'	String	Detector material: HPGe, NaI, CZT, LaBr3
configuration.detector.geometry	Column S 'Detector type'	String	Detector geometry: Coax, Planar, Semi-planar
configuration.detector.analyzer	Column T 'Analyser'	String	System analyzer: ORTEC DART, DSPEC, integrated
configuration.attenuators	Columns U, AG, AH	String	Attenuator material and the thickness in millimeters. Format Material:Thickness with semicolon delimiter between pairs: Cd:2.0;Pb:1.6
configuration.distance	Column W 'Distance cm'	Real	Source to detector distance in centimeters
supplementary.detector_size	Column BC 'Detector size and/or model'	String	Detector characteristics: 56 mm dia by 56 mm thick coaxial
supplementary.electronics	Column BD 'Acquisition electronics'	String	Measurement electronics: Commercial Analog NIM electronics
supplementary.measurement_geometry	Column BE:BM 'Measurement geometry'	String	Measurement geometry information

Pu_spectrum_metadata	Reference in IRDB_reference_spectra.xls	Data type and Format	Description
UID.spectrum	Unique ID		
UID.metadata	Unique ID to Pu_source_metadata		
configuration.detector.analyzer.number_of_channels	Read from spectrum file	Integer	Number of analyzer channels
configuration.detector.analyzer.gain	Read from spectrum file	Real	Gain of analyzer in keV/ch
configuration.detector.analyzer.offset	Read from spectrum file	Real	Offset of analyzer in keV
configuration.detector.analyzer.energy_range	Calculated from spectrum file	Real	Energy range of detector in the format "E1-E2 keV"
configuration.detector.fwhm	Calculated from spectrum file	Real	FWHM in keV at 208keV
configuration.acquisition.date	Read from spectrum file	String Date/Time	Date and time spectrum was acquired in UTC
configuration.acquisition.total_counts	Calculated from spectrum file	Integer	Total counts in spectrum
configuration.acquisition.real_time.seconds	Read from spectrum file	Real	Spectrum real time
configuration.acquisition.live_time.seconds	Read from spectrum file	Real	Spectrum live time
configuration.acquisition.dead_time	Read from spectrum file	Real	Spectrum dead time
configuration.acquisition.count_rate	Calculated from spectrum file	Real	Spectrum count rate

Pu_spectrum_counts_metadata	Reference in IRDB_reference_spectra.xls	Data type and Format	Description
UID.spectrum	Unique ID to Pu_spectrum_metadata		
configuration.acquisition.counts	Read from spectrum file	String	Comma-separated list of counts per channel, enclosed by brackets

Pu_spectrum_checksum_metadata	Reference in IRDB_reference_spectra.xls	Data type and Format	Description
UID.spectrum	Unique ID to Pu_spectrum_metadata		
spectra.md5	Calculated from spectrum file	String, 32 characters	

Pu_source_metadata	Reference in IRDB_reference_spectra.xls	Data type and Format	Description
UID.source	Unique ID		
certificate.identification	Unique identifier	String	Identifier of certificate: PIDIE.5, PIDIE.7, SRP.15, etc.
certificate.pu.reference_date	From certificate	String Date/Time	Reference date of certificate in UTC
certificate.pu.pu.238.value	From certificate	Real	Composition, units given in certificate.fraction_unit
certificate.pu.pu.238.uncertainty	From certificate	Real	Composition uncertainty
certificate.pu.pu.239.value	From certificate	Real	Composition, units given in certificate.fraction_unit
certificate.pu.pu.239.uncertainty	From certificate	Real	Composition uncertainty
certificate.pu.pu.240.value	From certificate	Real	Composition, units given in certificate.fraction_unit
certificate.pu.pu.240.uncertainty	From certificate	Real	Composition uncertainty
certificate.pu.pu.241.value	From certificate	Real	Composition, units given in certificate.fraction_unit
certificate.pu.pu.241.uncertainty	From certificate	Real	Composition uncertainty
certificate.pu.pu.242.value	From certificate	Real	Composition, units given in certificate.fraction_unit
certificate.pu.pu.242.uncertainty	From certificate	Real	Composition uncertainty
certificate.pu.am.241.value	From certificate	Real	Composition, units given in certificate.fraction_unit
certificate.pu.am.241.uncertainty	From certificate	Real	Composition uncertainty
supplementary.pu.mass.value	From certificate	Real	Pu mass in grams
supplementary.pu.mass.uncertainty	From certificate	Real	Pu mass sigma
supplementary.pu.content.value	From certificate	Real	Pu content
supplementary.pu.content.uncertainty	From certificate	Real	Pu content sigma
certificate.document	Certificate document name	String	Filename of certificate document, page number: HEU_CRM146.pdf, Page 2
certificate.separation_date	From certificate	String Date/Time	Separation date listed on certificate in UTC
certificate.fraction_unit	From certificate	String	Composition unit weight percent (wt%) or atom percent (at%)
certificate.uncertainty	From certificate	String	Absolute or relative uncertainty
certificate.uncertainty.number_of_sigma	From certificate	String	Number of sigma of uncertainty

MOX

MOX_measurement_metadata	Reference in IRDB_reference_spectra.xls	Data type and Format	Description
UID.metadata	Unique ID		
UID.source	Unique ID to MOX_spectrum_checksum_metadata		
sample.material.type	Read from spectrum file path	String	Material measured: MOX
sample.material.chemical_composition	Column Q 'Nature'	String	Chemical compound or physical form of the material: U3O8, UO2, UF6
sample.material.form	Column Q 'Nature'	String	Physical form of the material: powder, metal, solution
sample.composition.u.234.value	From certificate, decay corrected	Real	Weight percent (isotopic weight ratio)
sample.composition.u.235.value	From certificate, decay corrected	Real	Weight percent (isotopic weight ratio)
sample.composition.u.236.value	From certificate, decay corrected	Real	Weight percent (isotopic weight ratio)
sample.composition.u.238.value	From certificate, decay corrected	Real	Weight percent (isotopic weight ratio)
sample.composition.pu.238.value	From certificate, decay corrected	Real	Weight percent (isotopic weight ratio)
sample.composition.pu.239.value	From certificate, decay corrected	Real	Weight percent (isotopic weight ratio)
sample.composition.pu.240.value	From certificate, decay corrected	Real	Weight percent (isotopic weight ratio)
sample.composition.pu.241.value	From certificate, decay corrected	Real	Weight percent (isotopic weight ratio)
sample.composition.pu.242.value	From certificate, decay corrected	Real	Weight percent (isotopic weight ratio)
sample.composition.am.241.value	From certificate, decay corrected	Real	Weight percent
sample.mox.u_pu_ratio.value	From certificate, decay corrected	Real	Ratio of U/Pu in sample
configuration.detector.material	Column S 'Detector type'	String	Detector material: HPGe, NaI, CZT, LaBr3
configuration.detector.geometry	Column S 'Detector type'	String	Detector geometry: Coax, Planar, Semi-planar
configuration.detector.analyzer	Column T 'Analyser'	String	System analyzer: ORTEC DART, DSPEC, integrated
configuration.attenuators	Columns U, AG, AH	String	Attenuator material and the thickness in millimeters. Format Material:Thickness with semicolon delimiter between pairs: Cd:2.0;Pb:1.6
configuration.distance	Column W 'Distance cm'	Real	Source to detector distance in centimeters
supplementary.detector_size	Column BC 'Detector size and/or model'	String	Detector characteristics: 56 mm dia by 56 mm thick coaxial
supplementary.electronics	Column BD 'Acquisition electronics'	String	Measurement electronics: Commercial Analog NIM electronics
supplementary.measurement_geometry	Column BE:BM 'Measurement geometry'	String	Measurement geometry information

MOX_spectrum_metadata	Reference in IRDB_reference_spectra.xls	Data type and Format	Description
UID.spectrum	Unique ID		
UID.metadata	Unique ID to MOX_source_metadata		
configuration.detector.analyzer.number_of_channels	Read from spectrum file	Integer	Number of analyzer channels
configuration.detector.analyzer.gain	Read from spectrum file	Real	Gain of analyzer in keV/ch
configuration.detector.analyzer.offset	Read from spectrum file	Real	Offset of analyzer in keV
configuration.detector.analyzer.energy_range	Calculated from spectrum file	Real	Energy range of detector in the format "E1-E2 keV"
configuration.detector.fwhm	Calculated from spectrum file	Real	FWHM in keV at 208keV
configuration.acquisition.date	Read from spectrum file	String Date/Time	Date and time spectrum was acquired in UTC
configuration.acquisition.total_counts	Calculated from spectrum file	Integer	Total counts in spectrum
configuration.acquisition.real_time.seconds	Read from spectrum file	Real	Spectrum real time
configuration.acquisition.live_time.seconds	Read from spectrum file	Real	Spectrum live time
configuration.acquisition.dead_time	Read from spectrum file	Real	Spectrum dead time
configuration.acquisition.count_rate	Calculated from spectrum file	Real	Spectrum count rate

MOX_spectrum_counts_metadata	Reference in IRDB_reference_spectra.xls	Data type and Format	Description
UID.spectrum	Unique ID to MOX_spectrum_metadata		
configuration.acquisition.counts	Read from spectrum file	String	Comma-separated list of counts per channel, enclosed by brackets

MOX_spectrum_checksum_metadata	Reference in IRDB_reference_spectra.xls	Data type and Format	Description
UID.spectrum	Unique ID to MOX_spectrum_metadata		
spectra.md5	Calculated from spectrum file	String, 32 characters	

MOX_source_metadata	Reference in IRDB_reference_spectra.xls	Data type and Format	Description
UID.source	Unique ID		
certificate.identification	Unique identifier	String	Identifier of certificate: PIDIE.5, PIDIE.7, SRP.15, etc.
certificate.pu.reference_date	From certificate	String Date/Time	Reference date of certificate in UTC
certificate.pu.pu.238.value	From certificate	Real	Composition, units given in certificate.fraction_unit
certificate.pu.pu.238.uncertainty	From certificate	Real	Composition uncertainty
certificate.pu.pu.239.value	From certificate	Real	Composition, units given in certificate.fraction_unit
certificate.pu.pu.239.uncertainty	From certificate	Real	Composition uncertainty
certificate.pu.pu.240.value	From certificate	Real	Composition, units given in certificate.fraction_unit
certificate.pu.pu.240.uncertainty	From certificate	Real	Composition uncertainty
certificate.pu.pu.241.value	From certificate	Real	Composition, units given in certificate.fraction_unit
certificate.pu.pu.241.uncertainty	From certificate	Real	Composition uncertainty
certificate.pu.pu.242.value	From certificate	Real	Composition, units given in certificate.fraction_unit
certificate.pu.pu.242.uncertainty	From certificate	Real	Composition uncertainty
certificate.pu.am.241.value	From certificate	Real	Composition, units given in certificate.fraction_unit
certificate.pu.am.241.uncertainty	From certificate	Real	Composition uncertainty
certificate.mox.u.percent	From certificate	Real	U percent
certificate.mox.pu.percent	From certificate	Real	Pu percent
certificate.mox.u_pu_ratio.value	From certificate	Real	U/Pu ratio
certificate.mox.u_pu_ratio.uncertainty	From certificate	Real	U/Pu sigma
supplementary.pu.mass.value	From certificate	Real	Pu mass in grams
supplementary.pu.mass.uncertainty	From certificate	Real	Pu mass sigma
supplementary.pu.content.value	From certificate	Real	Pu content
supplementary.pu.content.uncertainty	From certificate	Real	Pu content sigma
certificate.mox.u.234.value	From certificate	Real	Composition, units given in certificate.fraction_unit
certificate.mox.u.234.uncertainty	From certificate	Real	Composition uncertainty
certificate.mox.u.235.value	From certificate	Real	Composition, units given in certificate.fraction_unit
certificate.mox.u.235.uncertainty	From certificate	Real	Composition uncertainty
certificate.mox.u.236.value	From certificate	Real	Composition, units given in certificate.fraction_unit
certificate.mox.u.236.uncertainty	From certificate	Real	Composition uncertainty
certificate.mox.u.238.value	From certificate	Real	Composition, units given in certificate.fraction_unit
certificate.mox.u.238.uncertainty	From certificate	Real	Composition uncertainty
certificate.document	Certificate document name	String	Filename of certificate document, page number: HEU_CRM146.pdf, Page 2
certificate.pu.240eff.value	From certificate	Real	240Pu effective
certificate.pu.240eff.sigma	From certificate	Real	240Pu effective sigma
certificate.separation_date	From certificate	String Date/Time	Separation date listed on certificate in UTC
certificate.fraction_unit	From certificate	String	Composition unit weight percent (wt%) or atom percent (at%)
certificate.uncertainty	From certificate	String	Absolute or relative uncertainty

certificate.uncertainty.number_of_sigma	From certificate	String	Number of sigma of uncertainty

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