Lab spectroscopy extension

*EPN-TAP mandatory & regular optional parameters are in italics in the first column (*the other ones are from the experimental spectroscopy and other extensions*)*

New parameters / ideas from workshop in dark red-brown

Usage in PDS_speclib service no longer consistent with column 3 are underlined in blue (would have to be changed also in the 2 DLR services)

Lab spectroscopy extension	**group related to:**	**Iterated from SSHADE and other proposals in Rome**	**Initial proposal from PDS_speclib implementation**
target_class	sample reference	'sample', constant	'sample', constant
target_name		Provides name of a meteorite, lunar sample, IDP, micrometeorite, etc from which the sample is extracted - empty otherwise, no local ID	Provides an ID of the sample. Introduces the name of a meteorite or a lunar sample when applicable.
alt_target_name		Alternative target names/ID only - can't be used to store extra info on sample identification	not used
sample_id		To provide name/ID of measured sample in local collection (agreed)	Currently included in target_name. Various parts of the same sample can be indicated and described in sample_desc (such as "Location A", etc)
producer_name	measurement origin	These two provide enough credits in the table (agreed)	provide reference to whom measured the sample
producer_institute			
instrument_host_name		same	Standard name of the lab/facility
instrument_name		same	Name of instrument (as in publications)
sample_classification	sample description	provides composition as group, class, sub-class, etc… of sample, concatenated in a hash-list (=> flexible searches with LIKE and %)	Provides composition as group, class, sub-class, etc… of sample, concatenated in a hash-list (=> flexible searches with LIKE and %)
		same	Name of mineral to be included
		same	Must include specification "meteorite" plus the meteorite type when applicable, as well as description of (main) mixtures ingredients
		same	Meteorite types as in Krot et al 2005. Dana or Struntz classification tags can be used for minerals.
		same	Minor/trace components are not welcome here (would multiply false alarms)
grain_size_min		Min/max defined somehow, left to data provider Proposed code for bulk = 99999	provide the particle size range in µm
grain_size_max		(max value not expected to be intensively used) Proposed code for bulk = 99999	A very large value (eg, >1000 µm) can be used locally in a service to identify bulk material - see if we define a code for this (-1 could do, but we also have to reserve a code for N/A)
? Sample_origin ?		*Need to have a separated Origin parameter ? E.g.: Natural/synthetic, etc, including "mixture"?* *The drawback is the need to check several parameters* *TBC*	Included in sample_classification
azimuth_min	environment parameters	complement incidence, emergence, and phase	Azimuth angle in degrees - see if negative values of angles can have a special meaning
azimuth_max		negative values for azi and phase have a special meaning?	
pressure		unit TBC	Experimental conditions, in bar and K. Unit bar is not recommended by VO practices, TBC

temperature		K	K
measurement_atmosphere		same	Description of experimental conditions, free string. Measurements under vacuum are indicated here with the word "vacuum".
measurement_type	relative to setup	Contains UCD for this type of spectrum	The type of measurement/scale (REFF, I_over_F, etc…) provided as a UCD (being discussed at IVOA)
geometry_type		same, see proposed list below	such as bidirectional, biconical, directional-hemispherical, etc - see if this list can be frozen (not likely) Can be a hash-list if composited from several spectral segments
spectrum_type		proposed to store measurement_type in clear, associated to a specific UCD - see proposed list below UCD proposal to be forwarded to IVOA (but doubtful…). The main benefit is to have a detailed description of complex measurements independent from UCDs (agreed)	Relies on measurement_type, but accuracy of UCDs is not excepted to reach this level
sample_desc	descriptions	free string describing the sample, its origin, and possible preparation	Free string describing the sample, its origin, and possible preparation (hash-list forbidden, as samples ID may contain # character)
setup_desc		same	Free string or hash-list describing the experimental setup if needed - may include Aperture (size of sample measured), etc
data_calibration_desc		same	Free string or hash-list describing data post-processing / calibration
thumbnail_url	std parameters with special use	provides a link to a small spectral plot for quicklook only in VESPA portal (larger plots to be provided as separated granules with dataproduct_type = im)	Provides a link to a small spectral plot - caution should be taken to have units / values readable in full size (will be reduced in VESPA portal)
datalink_url		Can contain a series of links to descriptive files providing extra information (image, text…)	Best solution to link descriptive files providing extra information (such as chemical analyses, samples images…)
Species		Use it to store a chemical formula (alt: a list of atoms) - TBD *Comment*: this parameter can be misleading if used only in some services / cases - will suggest that products not found do not exist at all	More for basic atm in obsevational data, not used here. See if usage can be enlarged (e.g., to InChiKeys) - but for minerals?
species_inchikey ?		Check if required/useful, TBC	
dataproduct_type		'sp' for spectra, but need for other values in SSHADE	'sp' for spectra
*spectral_range_min (& *_max)*		same	Provide spectral range as frequency in Hz (EPNCore standard)
*spectral_sampling_step_min (& *_max)*		same	Provide sampling step as frequency in Hz (EPNCore standard - mostly to support radio range)
*spectral_resolution_min (& *_max)*		spectral_resolution_min/max should instead provide | fq / Dfq | = | lam / Dlam | (agreed upon during the workshop, then checked to be consistent with other fields)	Initially provided Dfreq in EPNCore 2.0 (to be changed in next DaCHS mixin)
Other ideas:	A parameter to identify a source database in a compilation service (such as SSHADE, or PDS_speclib)	original_publisher may complement producer_name & producer_institute if required (from contributive work extension)	Uses producer_name & producer_institute to refer to original measurements (service_title + server name) is intended to track data from another EPN-TAP service — Use of ivoID of service is more secure and would support all VO services, TBC
	Photometric measurement sets?	TBD	not considered, although some are present
	Optical constants: ~ two associated spectral a single file, or one / complex type? Description / table should be identical	TBC	not considered

	Band lists: tables with characteristics and attributions - EPNCore is not necessarily the best solution, see later proposal	TBD	not considered

Proposed value lists, from SSHADE:

geometry_type (revised list)

direct, specular, bidirectional, directional-conical, conical-directional, biconical, directional-hemispherical, conical-hemispherical, hemispherical-directional, hemispherical-conical, bihemispherical, directional, conical, hemispherical, other geometry, unknown

PDS_speclib also contains:
biconical, off-axis
biconical, on-axis
biconical on-axis reflectance factor - this one is inconsistent
directional_hemispherical

spectrum_type - revised list (UCDs to be used in data files and for measurement_type)

Spectrum_type value	UCD (existing ones only)	Comment / proposed (but do not exist)
raw		xxx;stat.uncalib (if it means: raw data…)
transmission	phys.transmission	
absorbance	phys.absorption ??	phys.absorbance
normalized absorbance	phys.absorption;arith.ratio ??	phys.absorbance;arith.ratio
optical depth	phys.absorption.opticalDepth	
absorption coefficient	phys.absorption.coeff	
scattering coefficient		phys.scattering.coeff (proposed for atmospheric studies)
extinction coefficient	obs.atmos.extinction refers to an integrated quantity	phys.extinction.coeff (proposed for atmospheric studies)
optical constants	phys.refractIndex	
ATR transmission	phys.transmission	
ATR absorbance	phys.absorbance	
complex admittance		
complex impedance		
relative complex permittivity	phys.dielectric	
dielectric loss tangent		
relative complex permeability		
magnetic loss tangent		
bidirectional reflectance	phys.reflectance.bidirectional	= r = I/F Accepted Feb 2018
bidirectional reflectance distribution function	phys.reflectance.bidirectional.df	= r / μ0 = BRDF Weird, but agreed Feb 2018
radiance factor	phys.reflectance	= r = RADF = I/F Accepted Feb 2018
reflectance factor	phys.reflectance.factor	= r / μ0 = REFF Weird, but agreed Feb 2018
normalized reflectance	phys.reflectance;arith.ratio	Normalized to a std wvl (not with a coef)
albedo	phys.albedo	
normalized Stokes parameters	phys.polarization.stokes	(all)

normalized Stokes parameter Q	phys.polarization.stokes.Q	
normalized Stokes parameter U	phys.polarization.stokes.U	
normalized Stokes parameter V	phys.polarization.stokes.V	
normalized Stokes parameter I	phys.polarization.stokes.I	
polarization contrast	phys.polarization ??	phys.polarization.linear ?? =>reduced Pq
degree of linear polarization	phys.polarization.linear	phys.polarization.linear.total ??
polarization position angle	phys.polarization.rotMeasure ??	phys.polarization.angle??
degree of circular polarization	phys.polarization.circular	reduced Pv
thermal emission		
thermal radiance	phot.radiance	Can be reflected also (at least for observations)
thermal emittance		
thermal emissivity	phys.emissivity	
scattering intensity	~~phys.absorption ??~~	phys.scattering - seems required, with subcategories (crossSection, absorption, extinction, albedo, + possibly coefficient for atm studies - TBC)
differential scattering cross section	phys.atmol.crossSection; arith.diff ??	phys.scattering.crossSection ?? - Need arith.ang for angular distributions?
normalized differential scattering cross section	phys.atmol.crossSection; arith.diff;arith.ratio ??	phys.scattering.crossSection;arith.ratio ??
scattering cross section	phys.atmol.crossSection ??	phys.scattering.crossSection??
absorption cross section	phys.atmol.crossSection ??	phys.scattering.absorption.crossSection
extinction cross section	phys.atmol.crossSection ??	phys.scattering.extinction.crossSection
scattering efficiency factor	phys.absorption ??	phys.scattering.crossSection;arith.ratio (ratio of cross-section to the geometrical cross-section)
absorption efficiency factor	phys.absorption ??	phys.scattering.absorption.crossSection;arith.ratio
extinction efficiency factor	phys.absorption ??	phys.scattering.extinction.crossSection;arith.ratio
single scattering albedo		phys.scattering.albedo
Raman scattering intensity		phys.raman.scattering (lesser priority)
normalized Raman scattering intensity		phys.raman.scattering;arith.ratio (lesser priority)
Raman scattering coefficient		phys.raman.scattering.coeff (lesser priority)
Raman scattering efficiency		phys.raman.scattering.efficiency (lesser priority)
fluorescence emission		phys.fluo.emission (lesser priority)
normalized fluorescence emission		phys.fluo.emission;arith.ratio (lesser priority)
fluorescence emission efficiency		phys.fluo.emission.efficiency (lesser priority)

Band lists	spect.line.intensity spect.line.width spect.line;em.freq	Species: meta.id;phys.atmol Transition: meta.id;spect;phys.atmol.transition (seen in an astro service) or simply phys.atmol.transition ?

Comment: it is highly unlikely that such a detailed description can be supported with UCDs - they are not intended for this, although UCDs for some of these quantities are already defined. Raman and fluorescence related quantities are difficult to produce and have lesser priority.