

LineTAP

A Proposal for a Relational Model for Spectral Lines

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First time presented at the November 2020 Interop, restarting work after one year break

- Motivation and Goal
- Use cases
- Current state
- Some open questions
- short demo if time permits

- What we have now:
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 - VAMDC/XSAMS, very detailed data model, very complex.
- We propose a relational data model can be used via TAP
 - TAP/ADQL is already well known, no need to learn a new protocol → existing libraries, implementations
 - parameters selected from the VAMDC data model
 - if possible, keep a simple one-table data model
 - keep only parameters that are needed by most common use-cases

Main use case that drove the development so far:

"A user with a rough idea of the kind of physics in an emitting or absorbing region wants to identify a line in a spectrum."

Examples:

- Identifying a single line
- Getting properties of well-known lines
- Retrieving spectral lines for cross-identification
- Finding spectral lines for specific species

What has been/is being done up to now:

- Some use cases collected (more use cases are welcome!)
- Selected relevant quantities from the VAMDC data model, mapping to LineTAP
- Draft of IVOA Note being written (first working draft probably by June 2022)
- Prototype service implementation on GAVO-Dachs
- Prototype client being implemented in SPLAT-VO
- Adapting data model with experience from implementations and feedback from specialists → still need feedback!

Spectral Line quantities

Name [Unit]	Type	Description
title	text	Human-readable line designation.
vacuum_wavelength [Å]	float	Vacuum wavelength of the transition
vacuum_wavelength_error [Å]	float	Total error in vacuum_wavelength
method	text	Method the wavelength was obtained with
ion_charge	integer	Total charge (ionisation level) of the emitting particle.
mass_number	integer	Number of nucleons in the atom or molecule
upper_energy [J]	float	Energy of the upper state
lower_energy [J]	float	Energy of the lower state
inchi	text	International Chemical Identifier InChI.
inchikey	text	The InChi key (hash) generated from InChi
einstein_a	float	Einstein A coefficient of the radiative transition.
oscillator_strength	float	Oscillator strength of the radiative transition.
weighted_oscillator_strength	float	Weighted oscillator strength of the radiative transition
line_strength	float	Total absorption by a spectra line
xsams_uri	text	A URI for a full XSAMS description of this line.
line_reference	text	Reference to the source of the line data; this could be a bibcode, a DOI, or a plain URI.

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- How to refer to a molecule in a query?
 - InCHI/InChiKey are unique, not practical/human readable
 - Name, Formula - not always unique.
 - probably need extra columns for names/formulas, or use external service to convert to InCHI

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- Method - more detailed descriptions or just theory/experiment?
- do we need so many transition probabilities?
 - einstein A, oscillator strength, weighted oscillator strength, line strength
 - would einstein A coefficient be enough?

- Please take a look: <https://github.com/mmpcn/slapvamdc>
- LineTAP services at <http://dc.zah.uni-heidelberg.de/tap>
- Document is still full of "TO DO"s
- Comments and contributions are welcome
- Working draft probably in June 2022

Thank you!