LineTAP

A Proposal for a Relational Model for Spectral Lines

Margarida Castro Neves[1,2], Markus Demleitner[1,2], Jean-Michel Glorian[4], Nicolas Moreau[3]

[1]ARI, ZAH, Universität Heidelberg

[2]German Astrophysical Virtual Observatory

[3]Paris Astronomical Data Centre

[4]Institut de Recherche en Astrophysique et Planétologie

IVOA Interop November 2020

LineTAP proposal

- Motivation
- Goal
- Main use case
- Current state
- Some open questions

Motivation

- What we have now:
  - VO SLAP/SSLDM, very few services, and few clients.
  - VAMDC/XSAMS, very detailed data model, very complex.
- New version of SLAP/SSLDM: would it make things better?
- Why not create a relational data model, that is simple and can be queried by the TAP protocol?
  - TAP/ADQL is already well known, no need to learn a new protocol
  - existing libraries, already implemented in clients
  - good for users, data providers and programmers :)

Goal

Our goal is to have a simple data model, by

- collecting use cases from different areas
- selecting data quantities that cover most use cases (from the very detailed VAMDC data model)
- keep only parameters needed by most comon use cases
- if possible, keep an one-table data model

Use case

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."

- the first idea was to deal only with atoms and not to think about molecules
- but it seems that there are also some use cases using molecules, which brings more complexity
- more use cases are needed

Current state

What has been done up to now:

- Some use cases collected (need more!!!)
- Preliminary list of relevant quantities selected from the VAMDC data model
- Mapping from VAMDC Data model to LineTAP
- Draft of IVOA Note being written

Spectral Line quantities

column name	description
title	name of the species originating the line.
spectral_location	energy equivalent to wavelength in vacuum
spectral_error	integrated error for the spectral location
method	method the wavelength was obtained with
stoichiometric_formula	the symbol of the chemical element or the molecule formula
ion_charge	ionisation level
mass_number	mass number
upper_state_configuration	upper state configuration
lower_state_configuration	lower state configuration
upper_energy	energy of the upper state
lower_energy	energy of the lower state
inchi	chemical species inchi
inchikey	chemical species inchikey
einstein_a	Einstein A coefficient
oscillator_strength	oscillator strength of radiative transition
weighted_oscillator_strength	Weighted oscillator strength of radiative transition
line_strength	Total absorption by a spectra line
line_reference_doi	Digital Object Identifier of bibliography source
line_reference_uri	Web link to the publication

Some questions: Units and errors for numerical quantities

- VAMDC: wavelength type provides vacuum/air information, a numerical data type containing units and an accuracy data type
- we would prefer to have wavelength value(always in vacuum with a fixed unit) and wavelength error in different columns of a table.
  $\rightarrow$ ADQL User Defined Functions will be provided for conversion.
- Which unit to use as default? One idea is to use an Energy unit (J), but right now the majority wants to keep length (Angstrom or m)
- Errors: statistical, systematic, estimated, etc
  $\rightarrow$ for simplicity the best would be to provide a combined error (use cases?)

Some questions: Search for molecules

- Including molecules to the data model makes it more complex
- How to refer to a molecule in a query?
  - By name: (Water, Carbon Monoxide ...) - not unique
  - By formula: (H2O, CO) - not unique
  - by InCHIKey: unique, not human readable
- Add new tables in the LineTAP Data Model to map InChi to names and formulas, and ...
- Leave this to external service?

The IVOA Note draft

- Please take a look: https://github.com/mmpcn/slapvamdc
- Document is still in an early phase, full of "TO DO"s
- Comments and contributions are welcome
- We need more use-cases

Thank you!