IVOA DAL WG Running Meeting #13

Tuesday 12 July 2022 - 07:00 UTC - vconf

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Agenda:

1. LineTAP status
2. Other business

LineTAP status

- Working Draft: https://github.com/ivoa-std/LineTAP
- LineTAP - TAP view based based on VAMDC but focussed on most common use cases

Referring to a species

- easy for atoms, complicated for molecules
- NM: Complex in VAMDC for molecules - have a form that takes criteria and converts it into an inchi key to search. Could not find a representation for molecules.
- NM: Then becomes a two step process
- MCN: Need to have a inchi library. Either need the client to use the Inchi library (written in c) or need to have query in the protocol
- FLP: Doesn't VAMDC have a library of molecules
- NM: VAMDC only has those for the domains covered by VAMDC - there might be others in LineTAP that are not covered
- CV: Normally when searching in JPL, CDMS, first get molecular weight, then service returns the candidate molecules
- NM: Yes could be done with the VAMDC service
- MCN: Then LineTAP would need to have molecular weight
- CV: Astronomers will know weight but might not know formula/name
- MCN: Would a query by weight then produce a list of candidate molecules

- CV: Yes that would work
- FLP: Don't use weight, generally use names
- CV: In Cassis can find name of molecule or can find weight, could be very convenient
- MCN: There are some services which given a name return the inchi, formula, weight - but was very difficult to add to server. e.g. Name: water, Formula : H_2O
- JD: Are there examples of species that might not be in VAMDC
- NM: Very ionised atoms, or very complicated molecules might not be in VAMDC
- NM: Service list at https://portal.vamdc.org/vamdc_portal/nodes.seam - it is the most complete list
- MCN: Some synthetic lines are not in VAMDC
- FLP: We should start using VAMDC service for the conversion - this would cover 90% of use cases. Alternative is to do everything again!
- NM: VAMDC has a single file download for the full list
- MCN: Have to think about how to do it in LineTAP
- NM: Would have to standardise the query interface of the species DB as it is currently specific to VAMDC needs.

Selecting the most probable lines in a spectral range

- Which quantities are needed?
- CV: Problem with VAMDC is which lines to choose - too many lines which are important for an astronomer but need a spectroscopist to advise
- MCN: Would like to select the most probable lines
- CV: Selected lines with least uncertainty as the most common - not correct but a first filter
- MCN: Which values would help?
- CV: Good question but unsolved
- MCN: einstein A, line strength
- CV: Need will vary between communities
- CV: Statistical weight
- FLP: Need degeneracies of levels, so need info about the levels to work out what to include or not
- FLP: Big difference between LineTAP and SLAP is how levels are described
- MCN: Idea of linetap is for the service to precalculate the values rather than. providing lots of details
- JD: Can the probablity/popularity of a line be precalculated?
- NM: Know the most common lines requested, so could build a database of just the most 100-200 frequently used lines. Already have a short list of say 500 lines. Should be simple to do.
- MCN: Question is which criteria to use to find most popular
- CV: Don't care about the obvious lines, but the non-obvious ones that might be in the data, so might not be the right approach
- CV: Select with frequency, wavelength, energy ranges, einstein A and

strength to find lines
- NM: Selection with the number of atoms could be a useful filter - may not want high weight
- CV: Use these sort of criteria in radio - not sure of other fields
- NM: Two useful options: molecule weight and number of atoms
- FLP/NM: Not in VAMDC but can be calculated easily
- JD: (afterwards) could have the top 500 have a flag or a status value while still being part of a larger list

Best units to use

- Different communities, different units - conversion functions
- FLP: Suggest having standard conversion system
- MCN: Define a set of standard user defined functions
- FB: Is this for the response or the query or both?
- MCN: Primarily for the query - there are examples in the text
- MCN: Standard would be in angstrom but could convert to metres, frequency etc
- FLP: Would also need for response

Solids

- Questions in the interop on solids but not in scope for the current version

Other topics:

- Zero Point Energy:
  - FLP: Zero point energy - are you still planning to do this? It doesn't seem too useful for spectroscopy
  - MCN: We decided to not use it as we were not sure how to do it and it is not needed in our use cases

- References
  - FLP: IAU/exec discussion - VAMDC are able to provide bibliographic references for the data - this is important. Could this be supported in LineTAP?
  - MCN: Have one parameter which is the line reference - can add bibcode, DOI etc to this
  - FLP: Would that be enough?
  - NM: VAMDC is working with DOI and that has been sufficient. Tried having a second table with the references in results to allow for several

refs per loine, but found it was too complex. So now we provide only one ref in the results.
- CV: Could be many refs per line - theoretical, experiments
- GM: Could datalink be used to provide multiple refs?
- MCN: Need to discuss with Markus D.
- MCN However want to keep LineTAP in one table

- Quantum Numbers
  - FLP: Trickiest question is quantum numbers - need degeneracies
  - MCN: If Einstein A is high does that mean oscillation strength is high?
  - MCN: Had them all in LineTAP, but no need if redundant
  - CV: Different domains - IR know oscillator strength, Radio know einstein coeff
  - MCN: One better for emission, other for absorption
  - CV: Need an expert in IR or UV absorption to be involved.
  - MCN: We can find someone
  - MCN: If need both values, add as extra param (oscillator strength) to LineTAP, or if you convert would need quantum numbers
  - CV: Adding both sounds good. Maybe on some will not have the data though
  - MCN: In VAMDC many have one or the other and not both - probably depends on the community who made the DB

- Implementation
  - MCN: Expect most LineTAP implemtations to be VAMDC databases
  - NM: Not sure services would want to host two apps to serve data
  - GM: Has Markus implemented this in DACHS?
  - MCN: Yes there are two sample implementations but data is not highly interesting
  - NM: Have 5 DBS to mantain, don't want to add maintenance load