Questions, Comments and Answers following the presentation

Molecular line parameters
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Tristram: *The SPLATALOGUE is a database of atomic and molecular lines in the submm/mm regime used by ALMA. How does this data base relate to that of VAMDC? Does VAMDC contain this data?*

No, VAMDC does not contain the SPLATALOGUE data base. VAMDC contains the original JPL, CDMS, HITRAN databases, in particular it contains the latest data of those databases with full documentation about the origin of the data. There is currently an effort made by VAMDC in order to upgrade the SLAP protocol used by SPLATALOGUE and by IVOA. The protocol will then be implemented in VAMDC. This will allow VO tools to retrieve, analyze and compare data from both VAMDC and SPLATALOGUE.

Smette: What is the typical accuracy for molecular line parameters (wavelength, intensity) for molecules in optical and NIR ranges?

This question is difficult to respond to in a general matter. Spectroscopic data in the actual version (2016) of the HITRAN data base, for example, specify accuracies in a range from better than 10^{-8} cm $^{-1}$ up to better than 1 cm $^{-1}$, or even "unreported" for line positions. For line intensities, HITRAN has five accuracy levels that divide the uncertainty spectrum from better than 1% to anything $\geq$ 20% and another set of three categories where the level of accuracy is not quantified. In HITRAN the whole spectrum of accuracies is actually used for both, positions and intensities, but the accuracy of a particular transition depends very much on the molecule and on the individual band.
Let's take water as an example and look at transitions with wavelengths $\leq$2 µm: 80% of the intensity values have uncertainties of 10% or worse, but 4% of lines (all around 2 µm) belong to the highest accuracy class of 1% or better. As line positions are concerned, about 90% of lines have accuracies between 0.01 and 0.0001 cm $^{-1}$, but about 4% of water lines have an accuracy of between 0.1 and 1 cm $^{-1}$ only.
In general, most of the molecular line positions in the data base fall in the accuracy range between 0.01 and 0.0001 cm $^{-1}$. With respect to intensities, data on stable diatomics, such as CO, have a very high accuracy: 12% of the CO transitions belong to the class of highest intensity accuracy (< 1%) and only 0.2% to the lowest accuracy ($\geq$20%). Reactive species on the other hand are much less accurate. OH, for example, has 58% of the transitions in the lowest accuracy class ($\geq$20%) and 33% in the next higher level (< 20% and $\geq$10%).

Nave: *Comment: The problem of antiquity of the data is also the case for atomic data, as illustrated by the speaker's problem with finding an accurate wavelength for the Cd line at 325 nm.*