

SHORT TERM SCIENTIFIC MISSION (STSM) – SCIENTIFIC REPORT

The STSM applicant submits this report for approval to the STSM coordinator

Action number: CM1405

STSM title: MARVEL investigation of the high-resolution spectra of the H₂¹⁶O and ¹⁴NH₃ molecules

STSM start and end date: 01/17/2019 to 01/24/2019

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PURPOSE OF THE STSM/

Providing highly accurate (experimental quality) rotational-vibrational energy levels for small molecular systems has many applications in science (including astronomy) and engineering. Two particularly relevant molecules of astronomical and atmospheric interest are H₂¹⁶O and ¹⁴NH₃. Through previous collaborations between the ELTE and the UCL groups the high-resolution rovibrational transitions measured for the two molecules has been considered up to 2013 for H₂¹⁶O and 2015 for ¹⁴NH₃.

The purpose of this STSM was to consider all the new sources published up to 2019 containing experimental data for the two molecules mentioned, match the new experimental transitions to their counterparts available from accurate first-principles computations (the data used became recently available in the UCL group), complete and validate the databases of experimental transitions, and perform the new MARVEL analysis, using the latest version of the MARVEL code developed in Budapest, resulting in an extended set of highly accurate empirical rovibrational energy levels.

DESCRIPTION OF WORK CARRIED OUT DURING THE STSM

The work carried out during the STSM can be divided into the following steps:

1. Inclusion of the last remaining new sources in the MARVEL input file, joining the data sources created at UCL and Budapest and validating them against each other.
2. Validation of the rovibrational transitions and energy levels by comparing the newly obtained empirical (MARVEL) energy levels with their first-principles counterparts.
3. Creation of complete hybrid datasets of rovibrational energy levels, with appropriate labels used both by experimentalists and quantum chemists, up to 7500 cm⁻¹ for both molecules, which should facilitate the analysis of several new spectra available to the two groups.
4. Work on the manuscripts detailing the new results.

- 1) Most of the ground work was done prior to the STSM by the two groups, joining the datasets created required less effort than expected.
- 2) Validation of the data is always a time-consuming process but the experience gained by the two groups during the earlier analyses allowed progress to be made toward completion of the datasets. This has been achieved for both molecules by the end of the STSM.
- 3) Matching the highly accurate empirical energy levels with their much less accurate first-principles counterparts proved to be reasonably straightforward up to the 7500 cm^{-1} limit.
- 4) Great progress has been achieved toward completing the two manuscripts.

DESCRIPTION OF THE MAIN RESULTS OBTAINED

For both molecules we achieved the stated goal of the STSM, namely obtaining a new set of accurate empirical rovibrational energies for $^{16}\text{H}_2\text{O}$ and $^{14}\text{NH}_3$ and getting close to the completion of the manuscripts reporting about our new results. In fact, for both molecules we created a complete set of energy levels up to 7500 cm^{-1} , which contains almost exclusively MARVEL energy levels for $^{16}\text{H}_2\text{O}$ and mostly MARVEL levels for $^{14}\text{NH}_3$. The accuracy of the empirical rovibrational energy level sets should prove highly useful in several applications, including the assignment of newly measured spectra.

FUTURE COLLABORATIONS (if applicable)

Having completed the data analysis, we keep working on the two manuscripts. It is expected that the manuscripts will be submitted before the end of the Action.