Invited Lectures L

September 7, Friday, 9:00 – 10:30

Theoretical Simulation of Molecular Spectra for Astrophysical and Atmospheric Applications: Cool Stars, Brown Dwarfs and Extrasolar Planets

Sergei N. Yurchenko[1]

[1]Department of Physics and Astronomy, University College London, London, WC1E 6BT, UK, s.yurchenko@ucl.ac.uk

Most information on the Universe around us has been gained by astronomers studying the spectral signatures of astronomical bodies. Interpreting these spectra requires access to appropriate laboratory spectroscopic data as does the construction of associated atmospheric models. The spectral characterization of astrophysical objects such as cool stars, brown dwarfs and extrasolar planets, that are cool enough to form molecules in their atmospheres, requires fundamental data for all species that contribute significantly to their opacity. However, with a few notable exceptions such as water and ammonia, the existing molecular line lists are not sufficiently accurate or complete. Modelling planetary and stellar atmospheres is difficult as their spectra are extremely rich in structure and their opacity is dominated by molecular absorbers, each with hundreds of thousands to many billions of spectral lines which may be broadened by high-pressure and temperature effects. Despite many attempts and some successes in the synthesis of transition lists for molecular absorbers, reliable opacities for many important species are still lacking.

In this contribution I will present a new project, called ExoMol, which aims to systematically provide line lists for molecules of key astronomical importance. About 30 molecules have been selected to be those most likely to be present in the atmospheres of hot astronomical body like extra-solar planets, brown dwarfs and cool stars, where the opacity data is currently either not available, or else is inadequate for inclusion in accurate modelling. We are using first principles quantum mechanical methods and empirical tuning based on laboratory spectroscopic data and making extensive use of state-of-the-art computing. The line lists and other information about the project will be made available via the ExoMol website: www.exomol.com. A more detailed description of the aims, scope and methodology of the project can be found in the article [1].

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References

[1] J. Tennyson and S. N. Yurchenko, MNRAS (2012), in press; arXiv:1204.0124

Collision-Induced Spectroscopy

Lothar Frommhold

University of Texas, Austin, TX, U.S.A., frommhold@physics.utexas.edu

Even so-called infrared inactive gases (hydrogen, nitrogen,…) absorb infrared radiation strongly, if gas densities are sufficiently high. This so-called collision-induced absorption (CIA) may be thought of being a "supermolecular" process, which arises from a complex of two (or more) interacting atoms or molecules, instead of an individual molecule or monomer. Intermolecular van der Waals interactions generate transient dipoles and thus infrared spectra by the same mechanisms that are responsible for the van der Waals forces (mainly electron exchange, multipolar induction, dispersion force). CIA spectra are as common as the van der Waals forces themselves. Interaction-induced dipoles and their spectra are typically "weak" and often go unnoticed, but they increase quadratically with density (or even with higher-orders of density) and usually dominate observable spectra at high density. The leading linear term of virial expansions of spectral intensities represents "allowed" spectra (where they exist) and the higher-order terms arise from the interaction-induced processes of pairs, triples,… of interacting molecules. Interaction- induced properties are often called "collision-induced", but they occur as well in non- collisional molecular complexes; supermolecular complexes may be considered to be bound ("van der Waals molecules") or "dissociated" ($\rightarrow$ free collisional complexes). We consider here bound $\rightarrow$ bound, bound $\rightarrow$ free, free $\rightarrow$ bound, and (for the most part!) free $\rightarrow$ free optical transitions of binary and higher-order supermolecules. Astronomers dealing with systems such as solar and extra-solar planets, cool white dwarf stars, cool main sequence stars, so-called first stars (star formation), etc. take a special interest in CIA, which under many conditions is a major source of the opacities commonly encountered in such work; Earth-bound observations must often be corrected for collision-induced absorption in the atmosphere, etc., etc. Other applications are known in remote sensing and air pollution. Practical applications like these require tables of opacities arising from molecular pairs, such as H_2–H_2, H_2–He, H_2–H, H–He,… as functions of temperature (from ≈ 20 K to thousands of kelvin), and for frequencies from the microwave and far infrared regions to the visible (and even beyond). Laboratory measurements are limited to relatively small frequency bands and low temperatures (< several hundred kelvin) so that we decided to do extensive *ab initio* calculations. Such calculations proceed in two steps: 1. quantum chemical computations of induced dipole surfaces (IDS) and potential energy surfaces (PES), and 2. molecular scattering calculations with the molecular pair coupled to the electromagnetic field[1]. The resulting pair spectra are shown to be in close agreement with laboratory measurements where they exist. Extensive opacity tables for astrophysical applications are either available[2] or near completion. First steps have also been taken to deal with three-body and higher-order induction effects. In conclusion we mention similar experimental and theoretical work on collision-induced Raman spectra of gases, liquids and solids, and the virial expansions of various properties of dense gases (Clausius-Mossotti and Lorentz-Lorenz equations).

References

[1] L. Frommhold. Collision-induced Absorption in Gases. Cambridge University Press (1993 and 2006)

[2] C. Richard et al. New Section of the HITRAN database: Collision-induced absorption (CIA). J.Q.S.R.T. (2011), doi:10.1016/j.jqsrt.2011.11.004