2e OSUG Atelier Spectroscopie /

2nd Spectroscopy Workshop of the Grenoble Earth and Space Sciences Observatory

OSUG

Observatoire des
Sciences de l'Univers
de Grenoble

Tuesday 3 March, 2015

LGGE, Salle Lliboutry (Campus, 54 rue Moliere)

Organizers: Denis Testemale and Erik Kerstel

Programme OSUG 2e Atelier Spectroscopie / 2nd Spectroscopy Workshop

Tuesday March 3, 2015

LGGE, Salle Lliboutry (Campus, 54 rue Moliere, Saint-Martin d'Hères)

08:45	Coffee and Welcome		
09:00	Nicole Jacquinet	LMD/IPSL	GEISA: A key tool for atmospheric remote sensing applications
09:20	Raymond Armante	LMD/IPSL	GEISA: A key tool for atmospheric remote sensing applications
09:30	Alain Campargue	UJF-LIPHY-LAME	HITRAN et la constitution des listes de raies de l'eau, CO2 et méthane
09:50	Marie-lise Dubernet	Obs. Paris-LERMA	VAMDC: Introduction to the Virtual Atomic and Molecular Data Centre
10:10	Razvan Caracas	Lyon-Lab Geologie	WURM: web-based repository of computed physical data for minerals
10:30	Coffee (20')		
10:50	Bernard Schmitt	UJF-IPAG	GhoSST-SSHADE : bases de données en spectroscopies X-UV-Vis-IR-mm des solides
11:10	Alexandre Siminovici	UJF-ISTerre	XRAYLIB
11:30	Sarah Bureau	UJF-ISTerre	"Inductively Coupled Plasma - Atomic Emission Spectroscopy" et bases de données
11:40	Round Table Discussion (1h20')		
13:00	Lunch (1h00')		
14:00	End		

Abstracts

The GEISA spectroscopic database: a key tool for atmospheric remote sensing applications

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The accuracy in the scientific exploitation of operational mission measurements heavily relies, on the quality of the spectroscopy being used in the retrieval process

In this context, the ARA/ABC(t) group at LMD develops and maintains, since 1974 - celebrating its 40th birthday (*) last year -, the GEISA database (Gestion et Etude des Informations Spectroscopiques Atmosphériques: Management and Study of Atmospheric Spectroscopic Information; Jacquinet-Husson et al, JQSRT 112 (2011). GEISA has been at the heart of state-of-the-art developments in *spectroscopy* and *radiative transfer modelling* to meet the needs of the international *space agencies*, by collecting, archiving and distributing all the necessary inputs for atmospheric radiative transfer models.

The role of molecular spectroscopy in modern atmospheric research has entered a new promising perspectives phase for remote sensing applications (meteorology, climatology, chemistry) with the advent of highly sophisticated spectroscopic instruments. With the launch of high spectral resolution instruments like AIRS on board EOS-Aqua (2002), IASI on Metop-A (2006), and now on Metop-B (2012), GOSAT (2009) and Suomi NPP (2011) spectroscopic data appear to be at the root of the investigation of climate change providing an improved understanding of the different phenomena driving the atmospheric system.

To take up this challenge, GEISA is constantly evolving, taking into account the best available spectroscopic data. It comprises not only the line-by-line parameters database in the spectral range from 10^{-6} to 35,877.031 cm^{-1}, but also two additional sub-databases: infrared and ultraviolet absorption cross-sections, microphysical and optical properties of atmospheric aerosols.

GEISA is implemented on the CNES/CNRS/IPSL "ESPRI/Ether" scientific centre for research, data, products and distribution services WEB site (**), where all the archived spectroscopic data and related information can be handled through user friendly associated management software facilities. It is used on-line by more than 300 laboratories working in various domains like atmospheric physics, planetology, astronomy, astrophysics.

GEISA, together with the LMD radiative transfer model 4A (***) in its operational version 4A/OP, co-developed by LMD and Noveltis (****), have become CNES references for MetOp-A and MetOp-B and, as such, are involved, at CNES, Noveltis and LMD, in the spectral calibration activities of the IASI instruments -currently recognized as a radiometric reference by the Global Space-based Inter-Calibration System (GSICS).

In the frame of the 2014 GEISA release and the work in progress in the CNES-MENINGE scientific group for the future of the IASI instruments (IASI-NG), we will present the current content and planned evolution of each of the three sub-databases.

A emphasize will be given to quantify the quality of those parameters for targeted spectroscopic data and/or molecules, illustrated by results of validations (calculated minus observed biases and standard deviations) using comparisons between radiative transfer modelling 4A/OP with satellite or ground-based measurements). A specific focus will be presented on the near infrared, using comparisons to the high spectral resolution ground-based measurements of TCCON. Finally, feedback from Metrology groups and from groups developing remote sensing instrumentation on latest needs to improve the precision/accuracy of spectroscopic data will be given.

(*) : http://www.lmd.jussieu.fr/geisa2014/
(**) : http://www.pole-ether.fr/etherTypo/
(***) : http://ara.abct.lmd.polytechnique.fr/index.php?page=4a
(****) : http://4aop.noveltis.com/

Quelques mots sur la base de données HITRAN

et sur la constitution des listes de raies de l'eau, CO_2 et méthane

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La base de données HITRAN http://www.cfa.harvard.edu/hitran/ est largement utilisée dans de nombreux domaines notamment pour les applications atmosphériques et planétologiques. Ses principales caractéristiques seront résumées.

Dans une deuxième partie, nous donnerons un aperçu de la constitution actuelle des listes de raies auxquelles nous avons contribué (vapeur d'eau, dioxyde de carbone et méthane). La grande variété de sources de la littérature utilisées pour construire les bases de données de ces molécules sera illustrée et discutée.

Introduction to the Virtual Atomic and Molecular Data Centre (VAMDC): Consortium and e-infrastructure

Marie-Lise Dubernet,
Chair of Board of Director of the VAMDC Consortium

The "Virtual Atomic and Molecular Data Centre Consortium",(VAMDC Consortium, http://www.vamdc.eu) is a Consortium bound by a Memorandum of Understanding aiming at ensuring the sustainability of the VAMDC e-infrastructure built during 2 FP7-EU projects (2009-2014). The current VAMDC e-infrastructure inter-connects about 30 atomic and molecular databases with the number of connected databases increasing every year: some databases are well-known databases such as CDMS, JPL, HITRAN, VALD,.., other databases have been created since the start of VAMDC. The data can be queried, retrieved, visualized in a single format from a general portal (http://portal.vamdc.eu) and VAMDC is also developing standalone tools in order to retrieve and handle the data on a desktop. The VAMDC Consortium provides software and support in order to include databases within the VAMDC e-infrastructure. An exemple of current feature of VAMDC is the constrained environment of description of data that ensures a higher quality for distribution of data; a future feature is the link of VAMDC with evaluation/validation groups. The talk will present the VAMDC Consortium and the VAMDC e-infrastructure with its underlying technology, its services, its science use cases and its extension towards other communities than the academic research community.

The WURM project
A freely available web-based repository of computed physical data for minerals

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The WURM project is a database of computed Raman and infrared spectra and other physical properties for minerals. The calculations are performed within the framework of the density-functional theory and the density-functional perturbation theory. The database is freely available for teaching and research purposes and is presented in a web-based format, hosted on the http://www.wurm.info web site. It provides the crystal structure, the parameters of the calculations, the dielectric properties, the Raman spectra with both peak positions and intensities and the infrared spectra with peak positions for minerals. It shows the atomic displacement patterns for all the zone-center vibrational modes and the associated Raman tensors. The web presentation is user friendly and highly oriented toward the end user, with a strong educational component in mind. A set of visualization tools ensures the observation of the crystal structure, the vibrational pattern, and the different spectra. Further developments include elastic and optical properties of minerals.

GhoSST-SSHADE : bases de données en spectroscopies X-UV-Vis-IR-mm des solides

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Le service GhoSST, et sa future extension européenne SSHADE, concernent la mise à disposition de la communauté de plusieurs bases de données sur les propriétés spectroscopiques et physiques des solides (glaces, minéraux, matériaux organiques et carbonés, cosmomatériaux, …) d'intérêts planétologiques, astrophysiques mais aussi terrestres. Ce(s) service(s) fourni(ront) les données de laboratoire indispensables à l'analyse des nombreuses données d'observations spectroscopiques des surfaces planétaires et terrestre et du milieu interstellaire ainsi que pour les aérosols et poussières.

Je présenterai les données qui ont vocation à être stockées dans ces bases, le modèle de données SSDM sur lequel elles sont construites, ainsi que l'interface web de ces bases de données. Je présenterai ensuite le projet d'infrastructure européenne de bases de données, SSHADE, qui sera développée dans le cadre du programme EPN2020-RI.

An overview of the XrayLib utility

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"Quantitative estimation of elemental composition by spectroscopic and imaging techniques using X-ray fluorescence requires the availability of accurate data of X-ray interaction with matter. Although a wide number of computer codes and data sets are reported in literature, none of them is presented in the form of freely available library functions, which can be easily included in software applications for X-ray fluorescence. This work presents a compilation of data sets from different published works and an Xraylib interface in the form of callable functions [1, 2]. Although the target applications are on X-ray fluorescence, cross sections of interactions like photoionization, coherent scattering and Compton scattering, as well as form factors and anomalous scattering functions, are also available.
Xraylib provides access to some of the most respected databases of physical data in the field of X-rays. The core of Xraylib is a library, written in ANSI C, containing over 40 functions to be used to retrieve data from these databases. This C library can be directly linked with any program written in C, C++ or Objective-C. Furthermore, the Xraylib package contains bindings to several popular programming languages: Fortran 2003, Perl, Python, Java, IDL, Lua, Ruby, PHP and .NET, as well as a command-line utility which can be used as a pocket-calculator. Although not officially supported, Xraylib has been reported to be useable from within Matlab and LabView.
The source code is known to compile and run on the following platforms: Linux, Mac OS X, Solaris, FreeBSD and Windows". [3]

References:
[1] A. Brunetti, M. Sanchez del Rio, B. Golosio, A. Simionovici and A. Somogyi, "A library for X-ray matter interaction cross sections for X-ray fluorescence applications", Spectrochimica Acta B 59 (2004) 1725-1731.

[2] T. Schoonjans, A. Brunetti, B. Golosio, M. Sanchez del Rio, V. A. Solé, C. Ferrero and L. Vincze, "The xraylib library for X-ray—matter interactions. Recent developments", Spectrochimica Acta B 66 (2011) 776-784.

[3] Text from https://github.com/tschoonj/xraylib/wiki

ICP-AES et bases de données

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L'ICP-AES pour « Inductively Coupled Plasma Atomic Emission Spectroscopy » est une technique de spectroscopie ou l'échantillon est en phase liquide. Cette technique permet de quantifier des concentrations élémentaires pour un grand nombre d'éléments.

Une base de données est utilisée pour identifier les éléments présents dans une solution. Elle est composée des longueurs d'onde d'émission de chaque élément associée aux intensités relatives. Une autre base de données utilisée est « GeoRem » , celle-ci compile les données de matériaux de référence et permet de vérifier la justesse des analyses. Enfin les données acquises sur la machine sont archivée dans la base de données « VSDAdministrator ».