BENCHMARK CALCULATIONS FOR ELECTRON COLLISIONS WITH COMPLEX ATOMS AND IONS

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We will summarize the basic ideas behind the highly flexible B-spline R-matrix (close-coupling) method [1] for the treatment of atomic structure as well as photo- and electron-induced transitions in atoms and ions. Two essential refinements compared to the standard R-matrix approach are i) the removal of orthogonality restrictions, which allows for term-dependent, and hence non-orthogonal, orbital sets to represent both the bound and continuum one-electron orbitals, and ii) the use of B-splines as a universal and effectively complete set to generate the R-matrix basis. These features enable high accuracy in the target description, as well as a consistent treatment of the scattering system. Details and a list of applications can be found in a recent Topical Review [2].

Extensions of the method to the fully relativistic Dirac-Coulomb scheme and intermediate energies allow for an accurate treatment of heavy targets as well as a completely non-perturbative way to handle electron-impact ionization. Finally, systematically studying the convergence of the close-coupling expansion by increasing the number of both physical as well as pseudo-states is of critical importance for estimates regarding the accuracy of theoretical predictions.

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References

[1] O. Zatsarinny, Comput. Phys. Commun. **174**, 273 (2006)

[2] O. Zatsarinny and K. Bartschat, J. Phys. B **46**, 112001 (2013)

Future Laboratory Spectroscopy for Remote Sensing of Exoplanets

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At present, there are over 1500 confirmed exoplanets **(http://exoplanets.org/),** and dozens of these are being investigated to understand their atmospheric compositions and temperatures. Such studies rely on complete and reliable spectroscopic databases for a relatively small number of molecular species, but for a wide range of temperatures. The future needs and our prospects for meeting these through laboratory studies will be discussed.

Inner shell X-ray Data in AtomDB

Adam Foster, Randall Smith, Nancy Brickhouse, SAO

The Astro-H satellite will launch in 2015, providing unprecedented energy resolution for a satellite in the >3keV energy band. This will allow significant examination of the inner shell iron lines at 6.4-6.7 keV, as well as lines of nickel, chromium and manganese. We will discuss the issues raised by this process in terms of data generation and storage, and how the AtomDB project has tackled this and converting the new data into useful models for the community. In addition, we will discuss issues relating to the storage and application of uncertainties in atomic databases.

VAMDC databases and partners

Ulrike Heiter, Uppsala University, and VAMDC Consortium

The VAMDC Consortium is a consortium of Institutes and Research Institutions that share a common technical and political framework for the distribution and curation of atomic and molecular data.

About 30 databases have implemented the technical standards allowing a simultaneous data extraction in a common format. The databases are maintained at institutions in France, the UK, Sweden, Germany, Russia, Italy, Austria, and the USA. In addition, the VAMDC Consortium has partners in India, South Africa, Korea, Australia, Japan, and Brazil, who are promoting the use of the standards and the VAMDC databases in their regions. I will give some examples for the types of databases currently connected to VAMDC.

HITRANonline: An online interface for the HITRAN database

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We present recent progress in the development of a modern online interface to the HITRAN database[1] of spectral parameters for the modelling of atmospheric radiative transmission. This interface accesses a relational database backend (see the talk by Laurence Rothman at this meeting) which stores the HITRAN data and associated metadata in a flexible and extensible format which overcomes many of the limitations of the existing, 160-character fixed-width text-based format.

The HITRANonline interface will provide several improvements to existing methods for querying and obtaining HITRAN data, including:

- Visualization of data in the form of simple spectral plots
- Querying and output of data in user-specified units
- Customizable output formats, including HDF-5 and XSAMS
- User preference profiles (login required) with saved search history
- Bibliography with links to original sources, customised to search results
- An API for accessing HITRAN data programmatically along with associated software tools for manipulating it interactively within Python (see the talk by Roman Kochanov at this meeting).

In this presentation, we demonstrate the current status of the HITRANonline interface and discuss its advantages and its relation to the VAMDC infrastructure.

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[1] Rothman, L.S., I.E. Gordon, Y. Babikov, A. Barbe, D. Chris Benner, P. F. Bernath, M. Birk, L. Bizzocchi, V. Boudon, L. R. Brown, A. Campargue, K. Chance, et al., “The HITRAN 2012 molecular spectroscopic database,” *J. Quant Spectrosc. Radiat. Transfer* **130**, 4-50 (2013).

Application Programming Interface (API) for the HITRANonline web service. Current state and goals

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An Application Programing Interface (API) for HITRAN has been developed to allow users on their local machines much more flexibility and power. API is a programming interface for the main data-searching capabilities of the new “HITRANonline” web service (see Christian Hill's talk). It provides a possibility to query spectroscopic data from HITRAN in a flexible manner using either *functions* or *query language*. The API permits downloading, filtering, and processing the spectroscopic data given by “HITRANonline”. Thus the main goal is providing a tool that works locally with the data fetched from the main site.

The API is aimed to provide:

1) Line-by-line spectra and cross-sections
2) Dynamic calculation of partition sums using TIPS [1]
3) Synthetic spectra using various line shapes
4) Gas mixture spectra.

A nice feature of using the API is that it reduces the load on the HITRAN server and reduces requirements on bandwidth and operational memory.

Currently the API is a module written in Python and it doesn't use external libraries for data querying and processing. Adding a Matlab version of API is planned in near future. The API is designed to deal with data in multiple formats (ASCII, XSAMS, HDF5) and has a capability to work directly with XSAMS-formatted files using the API functionality.

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[1] A.L. Laraia, R.R. Gamache, J. Lamouroux, I.E. Gordon, L. S. Rothman. Total internal partition sums to support planetary remote sensing. Icarus 215 (2011) 391–400

Critical Evaluation of Data on Atomic Energy Levels, Wavelengths, and Transition Probabilities

Alexander Kramida, NIST

Current methods of critical evaluation of wavelengths, energy levels, and transition probabilities for atoms and atomic ions at the National Institute of Standards and Technology will be summarized.

The VAMDC infrastructure

Nicolas Moreau, Paris Observatory, and the VAMDC Consortium

The VAMDC consortium aims at providing a unified environment to access atomic and molecular data from various databases.
This interoperability between heterogeneous data sources is achieved through a dedicated infrastructure. It includes a common data exchange format called XSAMS, a registry, listing all the databases available, a web portal to query them and web services to transform data from XSAMS to any other format.

I will introduce all those elements and show how they simplify access to atomic and molecular data. Then I will briefly introduce a tool called Spectcol that, among other functionnalities, uses this infrastructure to extract and to merge Einstein and rate coefficients from different sources.

The VAMDC project and the lessons learned

Nikolai Piskunov, Uppsala University, and VAMDC Consortium

I will describe the motivation behind building the Virtual Atomic and Molecular Data Center (VAMDC), the history and arguments that led to the infrastructure we have today. I will also highlight the interaction between the data producers, databases, users and the VAMDC consortium and its impact on data consistency and general quality of services. Finally I will outline the deficiencies of the current system that will need to be addressed in the future.

The NIST Atomic and Plasma Databases

Yuri Ralchenko, NIST

I will present an overview of numerical and bibliographic atomic and plasma databases maintained at NIST. The Atomic Spectra database contains recommended and evaluated data on level energies, spectral lines and transition probabilities for almost all elements in the periodic table. The bibliographic databases on level energies and spectra lines, transition probabilities, and line shapes and broadening are updated regularly and currently contain several tens of thousands of papers. The plasma databases include contributions from the NLTE Code Comparison Workshops and an online time-dependent collisional-radiative code FLYCHK.

HITRAN Database Enhancements Fostered by VAMDC Collaboration

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The HITRAN molecular spectroscopic database [1] has been in existence since the 1970s, and was primarily focused on providing spectroscopic parameters that could be used in radiative-transfer codes modeling terrestrial atmospheric transmission or radiance. It has always been structured in a fixed-length ASCII format, where each record represented the crucial parameters of a transition (rotational, rovibrational, rovibronic).

The VAMDC program used the HITRAN database as one of the first test cases, and this has provided an impetus to cast HITRAN into a relational database structure. The new structure allows us to address many shortcomings of the old text-like structure. We briefly describe some of the advantages of the new structure. These advantages include: the ability and efficiency of including many more parameter sets (such as those required for planetary atmosphere applications), the ability to include longer fields (such as required for parameters with many significant figures or extended quantum assignments), the ability for the user to make complex queries of the database, the ease for the developers to perform validation checks on data, the capability to provide provenance of data, etc.

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[1] Rothman, L.S., I.E. Gordon, Y. Babikov, A. Barbe, D. Chris Benner, P.F. Bernath, M. Birk, L. Bizzocchi, V. Boudon, L.R. Brown, A. Campargue, K. Chance, et al., "The HITRAN 2012 molecular spectroscopic database," *J. Quant Spectrosc. Radiat. Transfer* **130**, 4-50 (2013).

Collisional Rovibrational Molecular Excitation: Calculation and Scaling

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Abstract

Reliable molecular collisional data are essential inputs in many astrophysical models, especially those of the interstellar medium where molecular gas resides. Therefore, calculations of rate coefficients for neutral-neutral collisional processes such as rotational and vibrational excitation are crucial and are currently underway for a variety of systems. Rate coefficients for many systems of astrophysical interest, however, cannot be explicitly calculated due to reasons including the lack of an available interaction potential energy surface or the required computational resources. Rate coefficients for these systems are then estimated using known values from other systems. A common approach to obtaining unknown rate coefficients is to use scaling arguments based on the reduced mass of the collision system. For example, the more easily calculated He-collider rate coefficients are used to predict those of the H_2-collider. Since rate coefficients depend sensitively on both the reduced mass and the interaction potential of the collision system, an analytic scaling approach based on both the reduced mass and the strength of the potential can be used to determine unknown rate coefficients. Through either this reduced potential scaling approach or via calculation, our collisional rate coefficients are produced in BASECOL, LAMDA, and stout formats for the modeling community.

VAMDC consortium - Technical and political organisation.

Carlo Maria Zwölf, Paris Observatory, and the VAMDC Consortium

During our talk we will present the organisation of the political and human aspects in the VAMDC consortium. After the presentation of the different boards and working groups, we will describe the adopted business model, while detailing how this has impact on the internal and external strategies. Finally we will highlight the interest for potential consortium newcomers in joining the VAMDC consortium.