Using VAMDC Resources for Education and Research

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Abstract

The use of the free, online resources provided by the Virtual Atomic and Molecular Data Centre in education and research in the field of astronomy, with a particular emphasis on spectroscopy is demonstrated. The interoperable data format and standardized data query language provided by this project facilitates the use of many different data sets in software to model, for example, the atmospheres of stellar and planetary atmospheres. Such databases, coupled with accessible website applications to make simple queries on them also provide a useful reference resource for atomic and molecular data in education.

1. Introduction

The Virtual Atomic and Molecular Data Centre (VAMDC, [1]) project has developed standards for data storage, searching and transmission which have been implemented on 22 major databases used by, amongst others, astrophysicists, astronomers, plasma physicists and atmospheric scientists. The ability to query many different databases simultaneously and retrieve data from them in a common format facilitates research in which such aggregation is otherwise laborious and time-consuming, whilst the conventions regarding data provenance (proper references and sources attached to each datum) ensure proper attribution and traceability of the data.

Furthermore, a valuable database of "meta-data" relating to atomic and molecular species is being built up as part of the VAMDC project. For example, isotope masses and abundances are readily obtained from a simple online query; the structure and thermodynamic data for molecular species are similarly obtained either through a webpage request or from within software able to post queries by HTTP.

2. Spectroscopic Simulation

The modeling of a molecular absorption spectrum requires data from potentially many different sources: the line intensities themselves are typically provided by one database (for example, HITRAN [2]); but the temperature-dependence of the spectrum requires knowledge of the molecule's partition function, the Doppler width of absorption lines depends on the molecular mass, molecular abundances may come from yet another source, etc.

The VAMDC services provide a simple interface (the VAMDC portal [3]) for obtaining the necessary data in a single XML document (XSAMS) which may be transformed into a more straightforward simple text format for input into a radiative transmission code. Alternatively, such a code can make direct queries of an available online service by HTTP. An example of such a code, written in the programming language Python, is provided.

3. Reference Data for Education

There is a need for atomic and molecular data for use in physical science education. Frequently, such data is provided in appendices to textbooks, in reference works, or by online resources such as Wikipedia. The standards established by the VAMDC project enable a common interface to be used to access such data online, and ensure that it is properly referenced.

The use of such online services in higher education is described and examples given.

Acknowledgements

References

[1] Dubernet, M.-L., et al., Virtual Atomic and Molecular Data Centre, *Journal of Quantitative Spectroscopy and Radiative Transfer* Vol. 111, pp. 2151-2159, 2010.

[2] Rothman, L. S., et al., The *HITRAN* 2004 molecular spectroscopic database, *Journal of Quantitative Spectroscopy and Radiative Transfer* Vol. 96, pp. 139-204, 2005.

[3] http://portal.vamdc.eu/vamdc_portal/

5. Equations

Below, you will find examples of two equations. You should use an equation editor of your word-processing program in order to include your equation(s). The equation number should be placed at the right side of the column and all equations should be consecutively numbered.

$$a^2 + b^2 = c^2 \qquad (1)$$

$$E = m \cdot c^2 \qquad (2)$$

6. Summary and Conclusions

After having finished your paper in your word-processing program, please create a respective pdf file out of the document. The correct page settings of 237 (height) x 180 (width) mm are included in the template document. **Please make sure that the generated pdf file actually has a page size of 237 x 180 mm.** This is the only way to guarantee the proper inclusion of your paper in the Copernicus Office database. Please note that you are asked to upload a pdf file during the abstract submission in Copernicus Office. No other file type than .pdf is accepted for the file upload. The actual citation header will be added automatically!

Acknowledgements

References

[1] Author, A., Author, B., and Author, C.: First example of a cited article title, First Example Journal, Vol. 1, pp. 1-100, 1999.

[2] Author, D. and Author, E.: Second example of a cited book, Example Publishing House, 2000.

[3] Author, F.: Third example of a cited conference paper, The Great Science Conference, 1–7 February 2001, Sciencetown, Sciencecountry, 2001.