

Note

# GPRD, a database for the spectral properties of diatomic molecules of atmospheric interest

P. Passarinho, M. Lino da Silva \*

*Centro de Física dos Plasmas, Instituto Superior Técnico, Av. Rovisco Pais, 1049-001 Lisboa, Portugal*

Received 14 October 2005; in revised form 19 December 2005

Available online 3 February 2006

For some years, spectroscopic data from diatomic molecules commonly found in low-pressure plasmas and planetary atmospheres has been compiled to improve the knowledge of the spectral properties of such mixtures. Up to very recently, the only available reference was provided by Huber and Herzberg's classic book on the constants of diatomic molecules [1]. Since then, two different Web-based databases, DiRef [2] and RADEN [3], provided compilations of references associated with the spectra of diatomic molecules, the latter already providing a limited amount of numerical data.

The GPRD (Gas and Plasma Radiation Database) database moves a step further, as it provides factual data—level-dependent spectroscopic constants, Klein–Dunham coefficients, Franck–Condon factors and  $r$ -centroids, electronic and vibronic transition moments, oscillator absorption strengths and Einstein coefficients, level-dependent and overall cross-sections for continuum transitions—and its associated references, allowing the user to simulate the relevant rovibronic transitions of the database diatomic molecules.

Although this database provides the scientific community with a novel and yet unique tool for retrieving the overall spectral properties of diatomic molecules rovibronic transitions, otherwise missing spectroscopic data is also provided for the simulation of atomic continuum radiation. The database is also linked to the most preeminent databases on atomic radiation (providing data on discrete and photoionization radiation processes) [4,5]. Finally, vibrationally dependent spectroscopic data for the simulation of discrete and continuum transitions is also provided for small polyatomic molecules (this is currently limited to the CO<sub>2</sub> molecule). The proposed data can be considered as complementary of data provided by the HITRAN [6]

database, regarding the simulation of the spectral properties for high-temperature gases and plasmas. In short, the database currently encompasses spectral data for the main isotopes of 14 atomic (H, H<sup>-</sup>, C, C<sup>+</sup>, C<sup>-</sup>, N, N<sup>+</sup>, N<sup>-</sup>, O, O<sup>+</sup>, O<sup>-</sup>, Ar, Ar<sup>+</sup>, Ar<sup>-</sup>) and 32 molecular species (H<sub>2</sub>, H<sub>2</sub><sup>+</sup>, H<sub>2</sub><sup>-</sup>, C<sub>2</sub>, C<sub>2</sub><sup>+</sup>, C<sub>2</sub><sup>-</sup>, CH, CH<sup>+</sup>, CH<sup>-</sup>, CN, CN<sup>+</sup>, CN<sup>-</sup>, CO, CO<sup>+</sup>, CO<sup>-</sup>, CO<sub>2</sub>, CO<sub>2</sub><sup>+</sup>, N<sub>2</sub>, N<sub>2</sub><sup>+</sup>, N<sub>2</sub><sup>-</sup>, NH, NH<sup>+</sup>, NH<sup>-</sup>, NO, NO<sup>+</sup>, NO<sup>-</sup>, O<sub>2</sub>, O<sub>2</sub><sup>+</sup>, O<sub>2</sub><sup>-</sup>, OH, OH<sup>+</sup>, OH<sup>-</sup>). For now, most of the transition probabilities dataset is issued from two Ph.D. Thesis which critically reviewed the available spectral data for C, N, and O containing diatomic species [7,8]. However further datasets, issued from several peer-reviewed sources, are scheduled to be provided in a near-future.

The GPRD database can be accessed online at the internet address <http://cfp.ist.utl.pt/radiation/>. This database is freely available to the overall scientific community, and only requires electronic registration to provide full access to the overall web-based data. The database follows a tree structure in which the user first chooses among atomic and molecular data, then selects the specific chemical species, and finally selects the type of required data (rovibronic levels, bound–bound, bound–free or free–free transitions calculations). The author has finally to chose which spectroscopic parameters he wants to retrieve (Klein–Dunham, Einstein coefficients, etc.), and is provided with a list of the available sets.

The engine used in the database has been developed using the SQL language, and the user interface is written in PHP. The spectroscopic data is provided in two different formats. The first one is a spreadsheet in the XML format, which can be opened with popular software such as Excel or OpenOffice. A XSL/CSS stylesheet has been added to allow online viewing of the spectral data. A simplified comma-separated (.csv) text file containing the spectroscopic data is also provided. Both formats include information

\* Corresponding author. Fax: +351 21 841 90 13.

E-mail address: [mlinodasilva@mail.ist.utl.pt](mailto:mlinodasilva@mail.ist.utl.pt) (M. Lino da Silva).

on the data units. The database program is currently being run on an Apache server.

Future updates of the database will include critical comments on the available spectroscopic data by the database managers. Comments from the general spectroscopy community will also be accepted, to allow users to select the most relevant and accurate spectroscopic data for their own needs. Moreover, a specific section of the database, featuring experimental spectra from atomic and molecular systems, is scheduled for development. This will allow critical comparisons between synthetic spectra (generated from the different available datasets) and measured spectra.

### Acknowledgment

The authors acknowledge F. Passarinho for his assistance and contributions in designing the page layout.

### References

- [1] K.P. Huber, G. Herzberg, *Molecular Spectra and Molecular Structure—IV. Constants of Diatomic Molecules*, Van Nostrand Reinhold, New York, 1979, see also the NIST website <<http://webbook.nist.gov/>>.
- [2] P.F. Bernath, McLeod S. DiRef, *J. Mol. Spectrosc.* (2001) 207–287, see also <<http://diref.uwaterloo.ca/>>.
- [3] L.A. Kuznetsova, *Spectrosc. Lett.* 20 (1987) 665–723, see also <<http://www.elch.chem.msu.ru/cgi-bin/raden/raden.cgi/>>.
- [4] W.L. Wiese, J.R. Fuhr, T.M. Deters, *J. Phys. Chem. Ref. Data* (1996), Monograph No. 7. see also <<http://physics.nist.gov/PhysRefData/ASD/index.html/>>.
- [5] The Opacity Project Team, *The Opacity Project*, vol. 1, Institute of Physics Publishing, Bristol and Philadelphia, 1995. see also <<http://cdsweb.u-strasbg.fr/topbase/topbase.html/>>.
- [6] L.S. Rothman, A. Barbe, D. Chris Benner, L.R. Brown, C. Camy-Peyret, M.R. Carleer, K. Chance, C. Clerbaux, V. Dana, V.M. Devi, A. Fayt, J.-M. Flaud, R.R. Gamache, A. Goldman, D. Jacquemart, K.W. Jucks, W.J. Lafferty, J.-Y. Mandin, S.T. Massie, V. Nemtchinov, D.A. Newnham, A. Perrin, C.P. Rinsland, J. Schroeder, K.M. Smith, M.A.H. Smith, K. Tang, R.A. Toth, J. Vander Auwera, P. Varanasi, K. Yoshino, *JQSRT* 82 (2003) 5–44, see also <<http://cfa-www.harvard.edu/HITRAN/>>.
- [7] C.O. Laux, *Optical Diagnostics and Radiative Emission of Air Plasmas*, Ph.D. Thesis, Stanford University, HTGL Report No. T-288, 1993.
- [8] M. Lino da Silva, *Simulation des Propriétés Radiatives du Plasma Entourant un Véhicule Traversant une Atmosphère Planétaire à Vitesse Hypersonique: Application à la planète Mars*, Ph.D. Thesis (in French), Université, Orléans, 2004. see also <<http://cfp.ist.utl.pt/radiation/Documents/>>.