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"Modelling of collision induced absorption spectra of H_2-H_2 pairs for the planetary atmospheres structure: The second overtone band"

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Final report covering of NASA funding of the project "Modelling of collision induced absorption spectra of H_2-H_2 pairs for the planetary atmospheres structure: The second overtone band"

The main objective of the proposal was to **model** the collision induced, second overtone band of gaseous hydrogen at low temperatures. The aim of this work is to assist planetary scientists in their investigation of planetary atmospheres, mainly those of Uranus and Neptune.

The recently completed extended database of collision induced dipole moments (C. Zheng, Ph.D. Thesis, MTU, 1997) of hydrogen pairs allowed us, for the first time, to obtain dipole moment matrix elements responsible for the roto-vibrational collision induced absorption spectra of H_2-H_2 in the second overtone band. Despite our numerous attempts to publish those data, the enormous volume of the database did not allow us to do this. Instead, we deposited the data on WWW site, at http://www.astro.ku.dk/~aborysow/data/. The final part of this work has been partially supported by NASA, Division for Planetary Atmospheres.

In order to use our new data for modelling purpose, we first needed to test how well we can reproduce the existing experimental data from theory, when using our new input data. Two papers resulted from this work, Y. Fu, C. Zheng and A. Borysow, 1999; and C. Brodbeck *et al.* 1999. The obtained agreement between theoretical results and the measurements appeared to be within 10–30%. The obviously poorer agreement than observed for the first H_2 overtone, the fundamental, and the rototranslational bands can be attributed to the fact that dipole moments responsible for the second overtone are much weaker, therefore susceptible to larger numerical uncertainties. At the same time, the intensity of the second overtone band is much weaker and therefore it is much harder to be measured accurately in the laboratory.

We need to point out that until now, no dependable model of the 2nd overtone band was available for modelling of the planetary atmospheres. The only one, often referred to in previous works on Uranian and Neptune's atmospheres, uses only *one* lineshape, with one (or two) parameter(s) deduced at the effective temperature of Uranus (by fitting the planetary observation). After that, the parameter(s) was(were) made temperature dependent according to some very simple relation. Summarising, no reliable temperature-dependent model has been available yet.

Our approach was a bit different from similar attempts done earlier, on account of the poorer agreement of theory with experiment. We needed to resort to some semi-empirical procedure. While we were in a favourable position to be able to rely on the physical input data, these, apparently, did not supply the most dependable predictions (simply because the results did not agree well enough with experimental data). On the other hand, the relative deviations between the theory and experiment were comparable at 77 and at 298 K. That fact indicated that theory is capable of predicting the temperature dependence of the absorption spectra well. We have thus chosen the "middle way". We have fitted the existing measurements with many 3-parameter lineshapes, in order to achieve the closest fit. Subsequently, we forced these parameters to follow the temperature dependence predicted by quantum mechanical theory. In this way not only we secured good reproduction of available experimental data, but we made sure that our predictions at temperatures *other* than those of experimental ones, will also be reliable. While making this fit, we took into account the considerably large experimental uncertainties (known), so that our predictions,

while following the "physical" temperature dependence, still fit the experimental data well within the error bars. The paper, entitled "Semi-empirical model of collision induced infrared absorption spectra of H_2-H_2 complexes in the second overtone band of hydrogen at temperatures from 50 to 500 K", co-authored by A. Borysow, J. Borysow and Y. Fu, has recently been submitted to *Icarus*. We are confident that this new model will be by far more useful than the model which existed until now. The fortran program will soon be available at
http://www.astro.ku.dk/~aborysow/programs/.

Principal investigator, A. Borysow, keeps updating the annual (unpublished) report listing all available computer models of CIA for planetary studies, entitled "Collision-induced absorption in the infrared: A data base for modelling planetary and stellar atmospheres", usually distributed at DPS Meetings or sent upon request; last edition: December 1998 (Borysow, unpublished, 1998). It is also available over the net, at www.astro.ku.dk/~aborysow/programs/.

All the relevant papers mentioned in this grant, with NASA, Division for Planetary Atmospheres acknowledged therein, have been enclosed with this report.

Refereed papers relevant to this project published, submitted, and in press (1998–1999)

(with NASA, Planetary Atmospheres Division acknowledged)

1. C. Brodbeck, J.-P. Bouanich, Nguyen-Van-Thanh, Y. Fu, and A. Borysow. Collision-induced absorption by H_2 pairs in the second overtone band at 298 and 77.5 K. *J. Chem. Phys.*, 110:4750, 1999.

2. Y. Fu, C. Zheng, and A. Borysow. First quantum mechanical computations of collision induced absorption in the second overtone band of hydrogen. *J. Quant. Spectrosc. Radiat. Transfer*, 1999, *in press.*

3. C. Brodbeck, J.-P. Bouanich, Nguyen van Thanh, and A. Borysow. The binary collision-induced second overtone band of gaseous hydrogen: Modelling and laboratory measurements. *Planetary and Space Sciences*, 1999, *in press* .

4. A. Borysow, J. Borysow and Y. Fu. Semi-empirical model of collision induced infrared absorption spectra of H_2-H_2 complexes in the second overtone band of hydrogen at temperatures from 50 to 500 K. *Icarus*, 1998, *submitted*; 1999, *resubmitted.*

Related refereed papers published in 1997–1998

(with NASA, Planetary Atmospheres Division acknowledged)

1. M. Gruszka and A. Borysow. Roto-translational collision-induced absorption of CO_2 for the atmosphere of Venus at frequencies from 0 to 250 cm^{-1} and at temperature from 200 K to 800 K. *Icarus*, 129:172–177, 1997.

2. M. Gruszka and A. Borysow. Computer simulation of the far infrared collision-induced absorption spectra of gaseous CO_2. *Mol. Phys.*, 93:1007–1016, 1998.

3. R. E. Samuelson, N. Nath, and A. Borysow. Gaseous abundances and methane super-saturation in Titan's troposphere. *Planetary & Space Science*, 45/8:959–980, 1997.

Conference contributions in 1997 – 1999 (abstracts)
(with NASA, Planetary Atmospheres Division acknowledged)

1. Yi Fu and Aleksandra Borysow, "Modelling of Collision-induced Absorption Spectra of H_2-H_2 Pairs for the Planetary Atmospheres Structure: The Second Overtone Band", 29th Annual Meeting of the Division for Planetary Sciences of American Astronomical Society, Cambridge, Massachusetts, July 28-August 1, 1997. Bull. of the AAS, vol. 29, p. 995 (1997). Poster presentation.

2. Claude Brodbeck, Jean-Pierre Bouanich, Nguyen-van-Tanh, Yi Fu and Aleksandra Borysow, "Collision induced absorption by H_2 pairs in the second overtone band at 298 and 77.5 K: Comparison between experimental and theoretical results", Symposium on "The Jovian system after Galileo. The Saturnian system before Cassini-Huygens". Nantes (France), Cite des Congres, May 11-15, 1998. Poster presentation.

3. Aleksandra Borysow, Yi Fu, Claude Brodbeck, Jean-Pierre Bouanich, and Nguyen-van-Thanh, "Collision-induced absorption by H_2 pairs in the second overtone band: comparison between experimental and theoretical results", 14th International Conference on Spectral Line Shapes, State College, Pennsylvania (USA), June 22-26, 1998. Poster presentation.

4. Aleksandra Borysow and Jacek Borysow, "Semi-empirical model of the CIA in the second overtone band of H_2 at 50 to 500 K"; *to be presented* at the 31st Annual Meeting of the Division for Planetary Sciences, AAS, Padova, 10–15 October, 1999.

Unrefereed documents distributed and made available by the author
(postscript files, numerical data and Fortran programs)

1. A. Borysow. "Collision–induced absorption in the infrared: A data base for modelling planetary and stellar atmospheres". A detailed report updated annually. Last update Dec. 1998. The paper is available in a postscript form at http://www.astro.ku.dk/~aborysow/programs/.

2. Our *ab initio* collision induced dipole moments of H_2-H_2 molecular complex database is made available at http://www.astro.ku.dk/~aborysow/data/ and the extended writeup (unpublished) describing the details of computations is now placed at http://www.astro.ku.dk/~aborysow/H2_dipole_CIA_LT/.
The dataset presented on WWW has been computed during years 1994-1997, and was aimed at being the starting point to compute high temperature CIA opacities for cool stellar atmospheres as well as the higher overtone bands.

3. A whole range of various FORTRAN computer programs, offering models of collision induced absorption (CIA) opacities for modelling of planetary atmospheres (outer planets, Titan and Venus) and cool stellar atmospheres ($T_{eff} \leq 4500$ K) has been recently placed at http://www.astro.ku.dk/~aborysow/programs/.
The programs are the result of 14 years of research leading to make models of CIA available for studies of planetary and stellar atmospheres. This new home page has now been linked to the Planetary Database Archives (PDS, PDS Atmospheres Node) database, among other Numerical Atmospheric models, see http://atmos.nmsu.edu/model.html.

Graduate students advised and graduated

During this period the PI advised, and graduated a Ph. D. student at the Michigan Technological University, Mrs. Yi Fu. Yi Fu received her Ph.D. degree for the work entitled "Molecular Spectroscopy in Gases", in April 1998. Her work was essential to the completion of this grant proposal, as documented by numerous publications.

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