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Modeling of collision induced absorption spectra of CO_2-CO_2 pairs for planetary atmosphere of Venus

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The objective of the proposal was to model the rototranslational, and the rotovibrational collision induced absorption spectral bands of importance for the radiative transfer analysis of the atmosphere of Venus.

The work has progressed, and is close to produce the first meaningful results. Our main task has been to compute the roto-translational (and, as a long term goal, also the rotovibrational) collision-induced absorption spectra of CO_2 pairs. The approach is not straightforward: whereas computational techniques to compute CIA spectra of small linear molecules exist, and were successfully applied to molecules like H_2 or N_2, they fail when applied to large molecules like CO_2. For small molecules one can safely assume that the interaction potential is isotropic. Same approximation does not work for CO_2, and when employed, it gives an incorrect band shape and only 50% of the CIA intensity.

We have started with examining the CIA spectral moments, to asses the significance of the effect of the anisotropy of the interaction potential, and to select the most suitable model for CO_2 pairs. We have been successful at that [1]. Currently, based on the information gathered in preliminary tests, we are close to the completion of computing the spectra. It needs to be mentioned that there have been no prior computations of that sort. Molecular Dynamics simulations, which we use, have been originally designated for liquids only, whereas our attempt is to apply them to the gas phase. At present, we have reached the agreement between the spectral moments obtained from Molecular Dynamics and from the independent code we used before [1]. We are thus confident about the computational tools we developed. Within these days we expect to obtain full RT CIA spectral band. We seem also to be very close in getting (by adjusting the overlap contribution to the induced dipoles) a good agreement between the computed, and the experimental spectral moments.

Our next goal is to reach same degree of agreement between the computed and experimental spectral profiles. Once it is reached, we'll be ready to run computations also at the temperatures of interest to Venus (i.e. up to 700K). Having mastered the numerical technique, we are confident that we will be able to deliver dependable model of CIA absorption spectra as a function of frequency and temperature. We will distribute that model, in a form of a FORTRAN computer program, as soon as it is ready, to all interested planetary scientists.

One publication, related to CO_2 CIA spectra, resulted from the last year NASA funding: "Spectral moments of collision-induced absorption of CO_2 pairs: The role of the intermolecular potential", by M. Gruszka and A. Borysow [1].

Related work

Few publications related to other planetary applications resulted from our last year research. Following publications have been completed with a partial support of the NASA grant. NASA support has been acknowledged in each of them and all the preprints are attached.

"Modeling of Collision–Induced Infrared Absorption Spectra of Pairs in the First Overtone Band at Temperatures from 20 to 500 K", by C. Zheng and A. Borysow, *Icarus*, in press, March 1995 [2].

"New analysis of the spectral moments of collision induced absorption in gaseous N_2", by M. Gruszka and A. Borysow, *Molecular Physics*, submitted, currently being revised [3].

"On the desymmetrization of the collision-induced roto-translational spectral profiles of pairs of freely rotating linear molecules", by A. Borysow and O. Ruehr, *Molecular Physics*, in press (1995) [4].

"Collision–induced absorption in the infrared: A data base for modeling planetary and stellar atmospheres", unpublished report updated semi-annually, distributed at various occasions, including the DPS Meetings, first edition: Oct. 1994 [5].

"Collision induced absorption of H_2–H_2 and H_2–He in the rotational and fundamental bands (0–6,000cm^{-1}) for planetary applications", by G. Birnbaum, A. Borysow, L. Frommhold and G. S. Orton, *Icarus*, to be submitted (1995) [6].

Conference Abstracts
(with NASA support acknowledged)

We presented three contributions at the XII International Conference on Spectral Line Shapes, Toronto, Canada, June 1994:
1. C. Zheng and A. Borysow,
"Rototranslational CIA spectra of H_2-H_2 at temperatures between 600 and 7,000 K";
2. M. Gruszka and A. Borysow,
"Spectral Moments of Collision Induced Absorption of CO_2 and N_2 pairs";
3. M. Moraldi and A. Borysow,
"Spectral moments for the absorption coefficient of CO_2–Ar pairs".
In addition, we presented a paper at the recent DPS Meeting, Washington, DC, October 1994:
4. A. Borysow and C. Zheng,
"Modeling of Collision–Induced Absorption Spectra of H_2-H_2 Pairs in the First Overtone Band", *Bull. of AAS*, vol. 26, no. 3, 1994, p. 1102.

References

[1] M. Gruszka and A. Borysow. Spectral moments of collision induced absorption of CO_2 pairs: The role of an interaction potential. *J. Chem. Phys.*, 101:3573, 1994.

[2] C. Zheng and A. Borysow. Modeling of collision–induced infrared absorption spectra of H_2-H_2 pairs in the first overtone band at temperatures from 20 to 500 K. *Icarus*, 112:??, 1994.

[3] M. Gruszka and A. Borysow. New analysis of the spectral moments of collision induced absorption in gaseous N_2. *Mol. Phys.: Research Note*, 1994, *submitted.*

[4] A. Borysow and O. Ruehr. On the desymmetrization of the roto-translational spectra of freely rotating linear molecules. *Mol. Phys.*, 1994, *submitted.*

[5] A. Borysow. Collision–induced absorption in the infrared: A data base for modeling planetary and stellar atmospheres. A detailed report updated bi-annually.

[6] G. Birnbaum, A. Borysow, L. Frommhold, and G. S. Orton. Collision induced absorption of H_2–H_2 and H_2–He in the rotational and fundamental bands (0–6,000cm^{-1}) for planetary applications. *Icarus*, 1995, *to be submitted.*