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Collision–induced absorption in the infrared: A data base for modelling planetary and stellar atmospheres*

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ABSTRACT

Accurate knowledge of certain collision-induced absorption continua of molecular pairs such as H_2-H_2, H_2-He, H_2-CH_4, CO_2-CO_2, etc., is a prerequisite for most spectral analyses and modelling attempts of atmospheres of planets and cold stars. We collect and regularly update simple, state of the art computer programs for the calculation of the absorption coefficient of such molecular pairs over a broad range of temperatures and frequencies, for the various rotovibrational bands. The computational results are in agreement with the existing laboratory measurements of such absorption continua, recorded with a spectral resolution of a few wavenumbers, but reliable computational results may be expected even in the far wings, and at temperatures for which laboratory measurements do not exist. Detailed information is given concerning the systems thus studied, the temperature and frequency ranges considered, the rotovibrational bands thus modelled, and how one may obtain copies of the FORTRAN 77 computer programs by e-mail. As well, one can download all programs mentioned in Tables I and II from http://www.astro.ku.dk/~aborysow/programs/.

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INTRODUCTION

Dense, neutral atmospheres, even those composed of nonpolar molecules, absorb infrared radiation in various rotovibrational bands that may be forbidden by dipole selection rules in the isolated molecules; weak new bands at sums and differences of rotovibrational transition frequencies also occur. Collision-induced absorption arises from intermolecular interactions of two (or more) molecules; it is a supermolecular process that has been studied in great detail in various dense gases, especially in hydrogen and mixtures of hydrogen and helium (Welsh, 1972); also in oxygen, nitrogen, methane, etc., and mixtures of such gases (Dagg, 1985; Borysow et al., 1987). Collision-induced *roto-translational* bands are known in the far infrared and microwave regions, and *rotovibrational* bands, including various overtone bands, exist in the infrared and visible regions of the electromagnetic spectrum (Frommhold, 1993). The astrophysical significance of CIA has long been recognised (Field et al., 1966; Trafton, 1964; Herzberg, 1952). Supermolecular absorption determines significant features of planetary atmospheres, such as the vertical temperature profile, the high-altitude haze distribution, and offers opportunities for the determination of abundance ratios of helium and hydrogen, and of ortho- and para-H_2. Such spectra are obtained in certain spectral bands by earth-based observations. Previous space missions (especially IRIS of Voyager I and II) as well as future ones (Infrared Space Observatory, NIMS of Galileo, and VIMS of Cassini) call for an extended data base of collision-induced absorption. Equally important are the collision-induced opacities for modelling the cool, dense stellar atmospheres. (Linsky, 1969; Borysow, 1995; Borysow, 1994).

For the analyses of such spectra, absorption profiles need to be known accurately as function of frequency, density and temperature for the molecular pairs (and, perhaps, triplets, etc.,) normally encountered in such atmospheres. Most significant information of that kind is obtained by laboratory measurements of the absorption by compressed gases, but the use of laboratory spectra for the modelling of planetary atmospheres is not straightforward. The problem is one of interpolating (and usually also extrapolating) the absorption coefficients measured in the laboratory at a number of fixed temperatures to the temperatures of the atmospheres, without sacrificing much of the precision of the measurement. Temperatures of interest to the planetary scientist do generally not coincide with temperatures that are conveniently maintained in the laboratory. More or less empirical interpolation procedures have been attempted over the years by various authors for certain molecular systems and bands of interest. However, the results thus obtained are often inconsistent with predictions based on the fundamental theory, especially where extrapolation to low temperatures is involved. In short, purely empirical procedures do in general not provide the most reliable input for the purpose.

In recent years, a new approach has been developed that is based on a numerical integration of Schrödinger's equation, using the most accurate dipole and potential models presently available as input for a rigorous computation of supermolecular absorption. For several important molecular systems (H_2–H_2 and H_2–He, for various RT and RV bands) the computational results thus obtained were shown to be consistent with almost all relevant laboratory measurements of such absorption spectra. In other words, a formalism exists which provides the most reliable basis for the computation of collision-induced absorption in various rotovibrational bands of molecular pairs, over a wide range of frequencies and temperatures, even where laboratory data do not exist; all computational results are consistent with the fundamental theory as well as with the measurements. Furthermore, dimer structures that could not be observed at the time in the laboratory, but were seen in the Voyager IRIS spectra (Frommhold et al., 1984; Schäfer and McKellar, 1990), have been explained in this way, thereby enhancing the potential for extracting significant new information from such spectra, see a recent monograph for details (Frommhold, 1993).

Significant progress has also been made to represent the computed collision-induced spectra in a form of relatively simple, analytical expressions that model the absorption quite accurately as function of frequency, gas density and temperature. The desirability for tractable analytical profiles for modelling of planetary atmospheres in the infrared has long been felt. For a number of systems and molecular bands of interest here, we have, therefore, presented the computational results in a form which permits a fairly rapid evaluation of the absorption coefficient as function of these parameters, even on small computers, without repeating elaborate quantum calculations. Simple FORTRAN 77 computer programs are available from the author that permit evaluation of the absorption in the infrared of several important molecular pairs commonly encountered in planetary and stellar atmospheres; e-mail inquiries are encouraged at aborysow@stella.nbi.dk.

Summarising, a relatively simple computational scheme has been created to duplicate almost instantaneously reliable absorption continua of common molecular pairs at nearly any temperature. The accuracy of the data thus obtained is as good as that of the best laboratory measurements of the kind presently available. The scheme permits substantial, dependable temperature and frequency interpolation and even extrapolation. Our models are most suitable for the low-resolution spectra. The bound-bound transitions, which are also present (with an exception of H_2-He pairs), can be computed only approximately (due to the isotropic potential approximation), and thus their models can be used as a low-resolution approximation.

BINARY SPECTRA

The computation of binary supermolecular spectra requires as input two functions of the intermolecular separation and orientation, namely the induced dipole moment and the intermolecular potential (Borysow and Frommhold, 1985). Intense research efforts have resulted in quite accurate, semiempirical models of the potential for many molecular pairs of interest in planetary atmospheres (Maitland et al., 1981); we use the most advanced model potentials presently available for the computations of the collision-induced absorption profiles.

Use of ab initio dipole surfaces

Highly developed quantum chemical methods exist to compute molecular and supermolecular properties from first principles. For example, attempts to compute induced dipole moments of molecular pairs are well known for the simpler atomic and molecular systems, such as H_2–H_2 and H_2–He. Recent work improved earlier results and considered the effects of electron correlation and vibrational averaging. Computed supermolecular wavefunction separate correctly into a product of H_2 wavefunctions for the separation $R \to \infty$. At the configuration interaction (CI) level, all atomic and molecular properties (polarizabilities and quadrupole moments) were found to be in agreement with the known values to within 1%. Various extensions of the basis sets employed have resulted in variations of the induced dipole moments of less than 1%. The precision of the best calculations of the kind may indeed be of that order (Meyer, 1985; Meyer and Frommhold, 1994).

Existing laboratory absorption spectra of H_2–H_2 and H_2–He pairs were closely reproduced by line shape computations based on the advanced ab initio dipole surfaces and models of the (isotropic) interaction potentials at all temperatures for which such measurements exist; see the examples shown in the "source references" listed in column 4 of Table 1. Under such conditions theory may be considered to be verified by measurement to the greatest possible extent. Such computations may thus be used to generate (or "predict") reliable absorption spectra at temperatures for which laboratory data do not exist. In this case, temperature interpolation of measurements is not a problem because theory states unambiguously all temperature dependencies and digital computers account rigorously for these. Spectral profiles have been computed over a wide range of temperatures in the roto-translational, fundamental and overtone collision-induced bands of H_2. These have been modelled with the help of the best analytical profiles presently known, for an easy duplication by the users of such data; relevant publications are given in the last column of Table 1 ("model" references).

We note that the line shapes are calculated using an exact quantum formalism and the most reliable input available. Vibrational dependencies of the interaction potential were for the first time accounted for in such work which have surprisingly strong influence on the resulting line shapes; these affect the asymmetry of the spectral profiles ("principle of detailed balance") which required a modification of standard model profiles in wide use (Frommhold, 1993). Isotropic interaction potentials are assumed which is (usually) a good approximation for the nearly spherical hydrogen molecules.

Use of the multipole-induced dipole model

In quantum chemical computations, pairs of bigger molecules (i.e., multi-electron molecules like N_2 and CH_4) have presently not been treated with the same precision as systems such as H_2–H_2 and H_2–He. One needs, therefore, alternative induced dipole functions for the modelling of the binary absorption based on quantum line shape computations. Fortunately, molecules other than H_2 and He have large polarizabilities and strong multipole moments so that the induced dipole sur-

Table 1: Collision-induced absorption of H_2-H_2 and H_2-He systems obtained from first principles. RT, F, O_2 and O_v stand for roto-translational band, fundamental band, first overtone and higher overtone band(s) of H_2, respectively. Column "model" lists available computer programs for modelling planetary and stellar atmospheres.

pair	band	frequencies (cm^{-1})	source Ref.	model Ref.	temperatures [K]
H_2-H_2	RT	0 – $\approx$ 2000	[1]	[2]	20 – 300
	RT	0 – $\approx$ 5000		[11]	600 – 7000
	F	$\approx$ 3500 – 5500	[3]	[4a]	20 – 350
	F	$\approx$ 2000 – 8000		[4b]	600 – 5000
	O_2	$\approx$ 5000 – 7000	[5]	[10]	(see Refs. [5,10])
	O_3	$\approx$ 11600 – 13000	[14]	[15]	20 – 500
	all bands	800–15,000	[16]	[17]	1000 – 7000
H_2-He	RT	0 – $\approx$ 2000	[6]	[7]	(see Refs. [6,7])
	F	$\approx$ 1000 – 8000	[8a]	[12]	18 – 7000
	F	$\approx$ 3500 – 5500	[8b]	[13]	20 – 300
	O_2 & O_v &"hot bands"	0 – $\approx$ 11000		[9]	18 – 7000
	all bands	800 – 15000	[16]	[17]	1000 – 7000

[1] (Meyer et al., 1989b)
[2] (Borysow et al., 1985)
[3] (Meyer et al., 1989a)
[4a] (Borysow, 1991; Borysow, 1993)
[4b] (Borysow and Frommhold, 1990)
[5] (Meyer et al., 1993) (temp. 20 – 300 K)
[6] (Meyer and Frommhold, 1986a; Birnbaum et al., 1987; Meyer and Frommhold, 1994) (temp. 20 – 300 K)
[7] (Borysow et al., 1988) (temp. 40 – 3000 K)
[8a] (Frommhold and Meyer, 1987; Moraldi et al., 1988) (temp. 20 – 300 K)
[8b] (Borysow et al., 1990)
[9] (Borysow and Frommhold, 1989) (temp. 18 – 7000 K)
[10] (Zheng and Borysow, 1995a) (temp. 20 – 500 K)
[11] (Zheng and Borysow, 1995b)
[12] (Borysow et al., 1989)
[13] (Borysow, 1992)
[14] (Fu *et al.*, JQSRT, 1999, *in press*, Brodbeck *et al.*, J. Chem. Phys., 1999, *in press*)
[15] (Borysow and Fu, Icarus, 1998, *submitted*)
[16] (Borysow *et al.*, 1997)
[17] ftp to stella.nbi.dk, anonymous, pass=your e-mail, cd /pub,
files: cia_dat_h2h2 and cia_dat_h2he

faces are closely described by the classical multipole induction model (Hunt, 1985). That description neglects the little known but generally relatively weak overlap- and exchange-induced dipole components, or it treats those spectral components arising from overlap induction as a small empirical correction. This approach has been very successful and permits a close reproduction of a number of roto-translational absorption spectra of binary systems involving like or dissimilar pairs of molecules like H_2, N_2, CH_4, and Ar. Complete references to the relevant source papers and the modelling for planetary work are given in Table 2.

Model line shapes

Spectroscopists have always found it useful to model measured line shapes with the help of analytical functions, such as Lorentzians or Gaussians, which may represent closely certain parts of spectral lines, such as the core or the distant wings. Collision-induced spectra are generally very diffuse, on account of the short collisional interaction time; as a consequence, the asymmetry arising from the principle of detailed balance can in general not be ignored. In response to these facts, "modified" desymmetrized functions have been proposed which represent collision-induced profiles somewhat more closely, but possibly not closely enough. It is, therefore, of interest that a number of simple, analytical models have been proposed especially for supermolecular spectra that are suitable for an efficient numerical computation, which reproduce measured and computed profiles of collision-induced absorption amazingly well. The most successful of these are the 3-parameter (Birnbaum and Cohen, 1976) "BC" model for multipole-induced lines, the 3-parameter "K_0" model for overlap-induced lines, and a combination of these, called the extended BC ("EBC") model which was constructed for special applications, such as the modelling of exact quantum line shape computations with great precision. These represent the exact profiles so well over an extended range of frequencies that in certain cases we found complex quantum line shape computations unnecessary, see (Borysow et al., 1985; Borysow et al., 1984), also (Moraldi et al., 1988) ("X&Y" functions) and (Birnbaum and Borysow, 1991) ("BB" lineshapes). Spectral components involving bound pairs (i.e., van der Waals molecules) require special consideration, but successful procedures have been developed for selected systems (Borysow and Frommhold, 1986a; Borysow and Frommhold, 1986b; Borysow and Frommhold, 1986c).

CONCLUDING REMARKS

For most analyses of the spectra of the planets and their big moons, collision-induced absorption of molecular pairs involving H_2, He, etc., must be known accurately over a wide range of temperatures and frequencies. By selecting the best dipole and intermolecular potential functions presently available, with the help of a rigorous quantum formalism, we have computed from first principles the collision-induced absorption spectra for several molecular pairs and the spectral bands listed in Tables 1 and 2. The results of the calculations were shown to be in close agreement with the laboratory measurements. We, therefore, feel that our quantum formalism offers the most reliable basis for the inter- and extrapolation of these laboratory data, with regard to both frequency and temperature.

Table 2: Collision-induced absorption for planetary atmospheres, based on a multipolar induction plus empirical dipole treatment. RT means roto-translational band. Column "model" lists available computer programs for modelling planetary atmospheres.

pair	band	frequencies (cm^{-1})	source Ref.	model Ref.	temperature [K]
CH_4–CH_4	RT	$0 - \approx 750$	[1]	[2]	50 - 300
H_2–CH_4	RT	$0 - \approx 1000$	[3,4]	[3]	50 - 300
H_2–N_2	RT	$0 - \approx 1000$	[5,6]	[5]	50 - 300
He–CH_4	RT	$0 - \approx 500$	[7]	[7]	40 - 350
N_2–N_2	RT	$0 - \approx 300$	[8]	[8]	50 - 300
N_2–CH_4	RT	$0 - \approx 600$	[9]	[10]	70 - 300
CH_4–Ar	RT	$0 - \approx 750$	[11]	[12]	70 - 300
H_2–Ar	RT	$0 - \approx 2000$	[13]	[14]	60 - 300
CO_2–CO_2	RT	$0 - \approx 250$	[15]	[16]	200 - 800

[1] (Borysow and Frommhold, 1987a)
[2] (Borysow and Frommhold, 1987b)
[3] (Borysow and Frommhold, 1986b)
[4] (Borysow et al., 1986)
[5] (Borysow and Frommhold, 1986c)
[6] (Dore et al., 1986)
[7] (Taylor et al., 1988) (FORTRAN program does not exist)
[8] (Borysow and Frommhold, 1986a; Borysow and Frommhold, 1987c)
[9] (Birnbaum et al., 1993)
[10] (Borysow and Tang, 1993)
[11] (Dore and Filabozzi, 1990)
[12] A. Borysow, unpublished work, 1993, see (Samuelson et al., 1997)
[13] (Meyer and Frommhold, 1986b)
[14] A. Borysow, unpublished work, 1994, see (Samuelson et al., 1997)
[15] (Gruszka and Borysow, 1998)
[16] (Gruszka and Borysow, 1997)

The exact computational results have been fitted to carefully selected analytical model profiles, functions of temperature and frequency, maintaining the numerical precision of the original work; computer codes for an efficient evaluation of these functions are available from the author.

Collision-induced absorption was recently recognised as an important opacity source in the atmospheres of cool stars (like brown dwarfs, M dwarfs or cool white dwarfs), for review see (Borysow, 1995; Borysow, 1994). **Attempts are currently being made to extend this data base to other molecular bands of hydrogen, and to higher temperatures of astrophysical interest**, using the approach described above.

We will continue to update the programs in our data bank, as soon as new models become available; we also plan to continue the practice of distributing FORTRAN **programs to all interested scientists modelling planetary and stellar atmospheres.** Presently, we consider *binary systems* of nonpolar molecules only. The current extent of the data base is best described by the information presented in Tables 1 and 2. The review of all computational efforts including many examples of the use of computer models related to CIA in pure hydrogen, and hydrogen-helium mixtures, for the planetary applications, can be found in (Birnbaum et al., 1996).

Extensive studies such as the ones mentioned above have shown that collision-induced absorption by binary systems is well understood and can be modelled accurately for atmospheric research, certainly for the simpler molecular systems at the temperatures encountered in the atmospheres of the outer planets and their big moons. However, it is well known that under certain conditions absorption by ternary complexes, indeed absorption by n-body complexes with $n > 2$, is significant. Ternary absorption is presently less well understood, albeit several simple facts are well known; the modelling of ternary spectral features is in its beginnings at best and may be important in some research related to planetary atmospheres, at a later time, ternary absorption of systems of nonpolar molecules, like H_2–H_2–H_2, might be similarly (but less rigorously) modelled.

Ternary collision-induced spectral components are discernible at high enough gas densities (see, for example, Moraldi and Frommhold (1989; 1993)) and also at frequencies and frequency shifts near zero (Poll, 1980; Lewis, 1985). The effects of high density are often significant, especially at the lower temperatures encountered in planetary atmospheres. These may be described in the form of a virial expansion, (Moraldi, 1990; Moraldi and Frommhold, 1992) in terms of powers of density, ϱ, with n-body components of intensity proportional to ϱ^n with $n = 2, 3, \ldots$ The 2-body coefficients are generally well known as this was seen above. The 3-body terms, on the other hand, may be estimated on the basis of a pairwise additive dipole model; 3-body coefficients have also been measured and modelled.

The low-frequency or "intercollisional" process mentioned is known to arise from the correlation of dipoles induced in subsequent collisions. Theoretically, it occurs even at the smallest densities in the form of a sharp "dip" of the absorption; with increasing density the dip grows broader, especially in the microwave and far infrared regions and at the H_2 $Q(J)$ branch.

In the near infrared, it has long been known that molecular bands of van der Waals molecules appear near the rotovibrational transition frequencies of the molecules involved, the spectroscopic signatures of molecular pairs bound by van der Waals forces. These dimer bands are to be contrasted with the diffuse bands of collision-induced absorption that arise from free pairs in collisional interaction. Absorption by bound pairs is due to the very same interaction-induced dipole components that determines collision-induced absorption. The spectral components of bound and free pairs are, therefore, more or less inseparable. In the roto-translational bands of the far infrared and microwave regions, dimer bands have only recently been seen in the laboratory (McKellar, 1990) and may be important for a novel determination of the hydrogen to helium abundance ratio in the atmospheres of the outer planets (Frommhold et al., 1984).

Line shape computations based on isotropic interaction potentials are very successful to model collision-induced spectra for most systems of interest for planetary atmospheres, including the summed contributions of bound dimers. However, high-resolution spectra will show dimer structures that cannot be modelled very well using the isotropic potential approximation, as was remarked above. One may in general expect that for not too anisotropic systems, spectra of high quality but limited resolution are obtainable by this approximation; the total intensity of the integrated dimer bands will be approximately correct. The positions of the rotovibrational dimer lines must be taken from laboratory measurements.

In case of systems consisting of considerably large molecules, like CO_2, an anisotropic potential needs to be used. We have done so, by running classical Molecular Dynamics simulations. By adjusting the unknown overlap component, we were able to reproduce the existing experimental results, and then model the RT CIA by CO_2 pairs (Gruszka and Borysow, 1998). Our new model uses different kind of model lineshape (BCBC), which combines the two BC lineshapes fitted to the low, and to the high part of the spectra (Gruszka and Borysow, 1997).

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