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**Astronomy
&
Astrophysics**

BASECOL2012: A collisional database repository and web service within the Virtual Atomic and Molecular Data Centre (VAMDC)

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ABSTRACT

The BASECOL2012 database is a repository of collisional data and a web service within the Virtual Atomic and Molecular Data Centre (VAMDC, http://www.vamdc.eu). It contains rate coefficients for the collisional excitation of rotational, ro-vibrational, vibrational, fine, and hyperfine levels of molecules by atoms, molecules, and electrons, as well as fine-structure excitation of some atoms that are relevant to interstellar and circumstellar astrophysical applications. Submissions of new published collisional rate coefficients sets are welcome, and they will be critically evaluated before inclusion in the database. In addition, BASECOL2012 provides spectroscopic data queried dynamically from various spectroscopic databases using the VAMDC technology. These spectroscopic data are conveniently matched to the in-house collisional excitation rate coefficients using the SPECTCOL sofware package (http://vamdc.eu/software), and the combined sets of data can be downloaded from the BASECOL2012 website. As a partner of the VAMDC, BASECOL2012 is accessible from the general VAMDC portal (http://portal.vamdc.eu) and from user tools such as SPECTCOL.

Key words. molecular data – virtual observatory tools – astronomical databases: miscellaneous – ISM: molecules – scattering – molecular processes

1. Introduction

Since the discovery of the first molecule in the interstellar medium (ISM) some fifty years ago, the number of detected molecules has steadily increased with time to more than 200 molecules nowadays[1]. The study of ISM molecules has various motives. First, it has been shown that a relatively rich chemistry can occur in the ISM, where the conditions are rather harsh in terms of temperature and density when compared to those on Earth. This chemistry mainly forms small diatomic molecules but also complex polyatomic molecules, the largest of them organic, which leads to the unanswered question of what might have been the role of ISM molecules in the terrestrial life appearance. Second, molecules are extremely important for probing the physical conditions of the gas, thanks to the fact that molecular lines are formed under particular temperatures and

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[1] E.g. see the list at www.astrochymist.org/ and www.astro.uni-koeln.de/cdms/molecules

densities that depend on the precise molecule structure and observed line. As a consequence, multifrequency observations can be used to reconstruct the physical structure of the studied object. However, in practice this is only possible if the so-called "collisional rate coefficients" are known. In the vast majority of the conditions present in the ISM, these coefficients are indispensable i) to convert an observed signal into a species column density and, therefore, abundance; and ii) to constrain the density and temperature of the emitting or absorbing gas. To this end, the molecular dynamics/quantum chemistry communities have been (and still are) extremely active in providing accurate collisional rate coefficients values (Dubernet et al. 2011).

With the advent of a new generation of heterodyne instruments possessing large instantaneous bandwidths, from the ground-based single-dish 30m IRAM to the Atacama Large Millimeter/submillimeter Array (ALMA) interferometer, and to the *Herschel* Space Observatory, the simultaneous observations of several molecular transitions is routine nowadays. In fact, unbiased spectral surveys are becoming a privileged tool for studying the chemical and physical structure of astrophysical sources (Bergin et al. 2010; Ceccarelli et al. 2010; Caux et al. 2011; Patel et al. 2011; Tercero et al. 2011; Ginard et al. 2012; Zernickel et al. 2012). Finally, the ever-increasing sensitivity of receivers will also lead to an increasing number of molecular lines to interpret. The huge investment in these new facilities, such as the *Herschel*-Heterodyne Instrument for the Far-Infrared (HIFI) (de Graauw et al. 2010) or the ALMA interferometer[2], therefore, makes the knowledge and availability of the collisional coefficients essential. In fact, in this context, having easy access to database of collisional coefficients has become more than an urgent need: it is a must.

The BASECOL database was first established at Besançon Observatory in 2002 in order to provide a compilation of references related to inelastic rate coefficients for atoms and molecules detected in ISM. The next version, BASECOL2005 (Dubernet et al. 2006) hosted at Paris Observatory (`basecol.obspm.fr`), was extended to include rate coefficients for some molecular species colliding with atoms and molecules. This version was accessible via its conventional web interface and via an automatic procedure for retrieving data (Moreau & Dubernet 2006a,b). The Leiden LAMDA database was established at the same time (Schöier et al. 2005).

BASECOL works on the concept of a collisional system comprising an atomic or molecular target species that contains internal structure and a projectile, which in general is assumed to be unstructured; however, this is not always the case, as seen in the discussion of collisions with H_2 in Sect. 2.2.1. The temperature used for the rate coefficients is the relative translation of the two colliders, while the target states are generally treated as being fully resolved.

Since the previous editions of BASECOL, fitted functions for many available rate coefficients have been added, collisional systems involving electrons have been included, and there have been continuing updates of the database with the latest published results for collisional systems of interest. However, the greatest conceptual change is the implementation of BASECOL2012 within the Virtual Atomic and Molecular Data Center[3] (Dubernet et al. 2010; Endres et al. 2011; Rixon et al. 2011).

The primary goal of the BASECOL database is to provide a standard repository of collisional rate coefficients for use by the scientific community. To ensure data quality, inclusion in BASECOL requires the team to critically evaluate any input data by reading the relevant papers and, when necessary, communicating with the original authors. Currently, BASECOL provides collisional data sets as originally published only and archives of earlier datasets for each given collisional system, thus providing long-term preservation of the data. For guidance to users, BASECOL indicates some sets as "recommended" based on an evaluation by the BASECOL team.

It should be noted that at present BASECOL does not contain experimental rate coefficients because those data are rarely obtained directly. Indirect measurements, such as line-broadening coefficients, are not relevant to BASECOL since it is hard to extract accurate collisional excitation rate coefficients from such measurements, see Drouin et al. (2010), Krupnov (2010),Wiesenfeld & Faure (2010), and finally Drouin & Wiesenfeld (2012) as an illustrative example. Nevertheless, indirect measurements of line broadening, line-shifting coefficients, or bound states of Van der Waals systems can give an assessment of the accuracy of some regions of the potential energy surfaces used in the heavy particle scattering calculations.

The database has a "Data" section that includes: a) Collision browser or search engine sections that give access to the collisional systems linking to collisional rate coefficients combined with experimental spectroscopic information and a brief description of the theoretical methodology used. b) Information on the energy levels used in the molecular dynamics calculations: this section is aimed at theoreticians who want to reproduce the rate coefficient calculations.

A "Bibliographic" section provides access to the bibliographic databases, and the "Tools" section provides tools that might be of interest to the astrophysical community, in particular the SPECTCOL tool (Dubernet et al. 2012; Dubernet & Nenadovic 2011) as well as some code packages to handle BASECOL data sets. A "Submit new data" section provides instructions about how to submit new collisional data sets. A "Publication" section contains publications associated to BASECOL, i.e. reviewed papers, proceedings, etc. The "Field news" section is meant to display information on current developments and future needs, the "Support" section provides information about how to register to the basecol-user list.

2. Overview of the BASECOL database

2.1. A bibliographic database on molecular energy transfer

Currently there are a total of 829 references in the bibliographic database, which is updated regularly. These references are mainly linked to the collisional data sets entered in BASECOL. They range from purely theoretical papers on dynamical or quantum chemistry methods to papers describing potential energy surfaces, collisional cross sections, and rate coefficients. In addition to a standard bibliographic search engine, a search via in-house keywords is provided since all papers have been indexed with keywords relevant for the inelastic collisions contained in BASECOL. Whenever possible, links to the web pages that have the original publications or to the SAO/NASA Astrophysics Data System (ADS) are also provided. The resulting citations can be extracted in BibTeX format.

2.2. Collisional systems

The BASECOL2012 database gathers and keeps information on collisional systems. This means that for a given collisional system, the users have access to sets calculated by different authors

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[2] `http://www.almaobservatory.org/`
[3] `www.vamdc.eu`

or by the same authors at different times. BASECOL2012 has the policy of not scaling the collisional rate coefficients of molecule-He systems and pretending that such scaled data can replace the corresponding molecule-H_2 data. It also does not scale a given neutral-neutral system to mimic another isoelectronic system. BASECOL2012 directly gets its spectroscopic data dynamically from the CDMS, JPL, HITRAN databases and keeps their own version. BASECOL2012 keeps a version of its own internal data sets. BASECOL collisional data allows for the possibility of state-to-state rate coefficients including transitions in a structured collider. Such a possibility is rich from the physical point of view, but might both complicate the lives of users and be considered as a feature of BASECOL. Therefore Sect. 2.2.1 provides the necessary explanations and recommendations. All these aspects define the difference between the BASECOL2012 and the LAMDA (Schöier et al. 2005) databases.

Another feature of BASECOL arose because users encountered difficulties choosing between different collisional sets for a given system, therefore a "recommended" mention is added to BASECOL2012 (see Sect. A.7). A long-lasting demand on BASECOL has been to provide combined collisional and spectroscopic data in the format used by the radiative transfer code RADEX (van der Tak et al. 2007), which is also used by the LAMDA database (Schöier et al. 2005). Therefore, BASECOL2012 has added this new feature in the "Radiation/Collision" section of the collisional sets. Table A.1 summarizes the information available for each collisional set.

2.2.1. Rate coefficients

The collisional rate coefficients provided by BASECOL are state-to-state rate coefficients, effective rate coefficients, and thermalized rate coefficients, each of which is defined below. In most cases state-to-state (de-)excitation rate coefficients are obtained at a given temperature from Boltzmann thermal averages of the calculated state-to-state inelastic cross-sections obtained on a grid of kinetic energies E:

$$R(\alpha \rightarrow \alpha'; \beta \rightarrow \beta')(T) =$$
$$\left(\frac{8}{\pi\mu}\right)^{1/2} \frac{1}{(k_B T)^{3/2}} \int_0^\infty \sigma_{\alpha \rightarrow \alpha'; \beta \rightarrow \beta'}(E) \, E \, e^{-E/k_B T} \mathrm{d}E, \quad (1)$$

where k_B the Boltzmann constant, μ the reduced mass of the colliding system, and (α, β), (α', β') represent the initial and final levels of the target (α) and collider (β)) species. Therefore a typical BASECOL rate coefficient table is composed of the following items: Cols. 1 and 2 contain the initial α and final α' levels of the target, Cols. 3 and 4 contain the initial β and final β' levels of the collider, the subsequent columns give the state-to-state rate coefficients (Eq. (1)) at different temperatures.

These state-to-state collisional rate coefficients follow the principle of detailed balance, and reverse rate coefficients $R(\alpha' \rightarrow \alpha; \beta' \rightarrow \beta)(T)$ can be obtained from forward rate coefficients by the usual formula:

$$g_{\alpha'} g_{\beta'} e^{-\frac{E'_{\text{int}}(\alpha')}{k_B T}} e^{-\frac{E'_{\text{int}}(\beta')}{k_B T}} R(\alpha' \rightarrow \alpha; \beta' \rightarrow \beta) =$$
$$g_\alpha g_\beta e^{-\frac{E_{\text{int}}(\alpha)}{k_B T}} e^{-\frac{E_{\text{int}}(\beta)}{k_B T}} R(\alpha \rightarrow \alpha'; \beta \rightarrow \beta'), \quad (2)$$

where g_α and g_β are the statistical weights related to the ro-vibrational levels of the target and collider, respectively, and the different E_{int} are the ro-vibrational energies of the species.

When the collider is an electron or an atom whose internal energy does not change during the collision, the state-to-state

(de)-excitation rate coefficient is Eq. (1) with $\beta = \beta' = 1$. For ISM studies, the usual atomic colliders are He, H, H^+, whose internal states do not change during the collision for kinetic energies relevant to ISM studies.

When the collider is a molecule, such as H_2, no such simplification occurs rigorously because the first transition in the rotational levels of para–H_2 and ortho–H_2 occurs around 354 cm^{-1} and 587 cm^{-1}, respectively. Nevertheless, except for the latest H_2O–H_2 calculations of Daniel et al. (2011, 2010) and Dubernet et al. (2009), where excitation of $j(H_2) = 2, 3, 4$ are considered, and for the SiS-H_2 system (Kłos & Lique 2008), HNC–H_2 (Dumouchel et al. 2011), and CN$^-$–H_2 (Kłos & Lique 2011) where rate coefficients with $j(H_2) = 2$ were provided, nearly all published calculations do not allow excitation of H_2, thereby fixing H_2 in its lowest para ($j = 0$) and ortho ($j = 1$) states. Within this approximation, which is usually but not always justified in the ISM, the state-to-state (de)-excitation rate coefficient is Eq. (1) with $\beta = \beta' = 1$ as for atoms.

State-to-state rate coefficients that include excitation of the colliding H_2 (Daniel et al. 2011, 2010; Dubernet et al. 2009) are not directly usable in the current astrophysics radiative transfer codes since these codes do not explicitly consider excitation of the collider. In this case it is necessary to use the so-called effective rate coefficients $\hat{R}_\beta(\alpha \rightarrow \alpha')$, which are given by the sum of the state–to–state rate coefficients (Eq. (1)) over final collider states, β' for a given initial β:

$$\hat{R}_\beta(\alpha \rightarrow \alpha')(T) = \sum_{\beta'} R(\alpha \rightarrow \alpha'; \beta \rightarrow \beta')(T). \quad (3)$$

These effective rate coefficients do not follow the principle of detailed balance, so both excitation and de-excitation rates should be calculated explicitly. In BASECOL the effective rate coefficients are clearly identified as "Effective" and the table's entry for the collider initial level indicates the β level of Eq. (3), while the collider final level is meaningless and is currently set equal to the initial level for convenience.

Finally, de-excitation rate coefficients for a thermalized collider can be obtained by averaging over the initial ro-vibrational levels of the collider:

$$\overline{R}(\alpha \rightarrow \alpha')(T) = \sum_\beta \rho(\beta)\hat{R}_\beta(\alpha \rightarrow \alpha')(T) \quad (4)$$

with $\rho(\beta) = g_\beta e^{-\frac{E_{\text{int}}(\beta)}{k_B T}}/Z$, where $Z(T)$ is the partition function obtained as sum over the β states. Such rate coefficients follow the principle of detailed balance.

For colliders having ortho/para species such as H_2, the user will consider the two species as independent in most cases. It should be noted that quasi-classical calculations (QCT) calculations, such as those of Faure et al. (2007b), directly calculate the rotational de-excitation rate coefficients of H2O by thermalized ortho/para H_2 considered as separate species. In BASECOL the thermalized rate coefficients are clearly identified as "Thermalized" and the entries for the collider's initial and final levels are meaningless. They are always denoted the $\beta = \beta' = 1$ level for convenience.

It has been found that for all collisional systems being studied the state-to-state or effective rate coefficients with $j(H_2) = 1$ are always higher than those with $j(H_2) = 0$, with the exception of excitation of the negative ion CN$^-$ (Kłos & Lique 2011) where there are no significant differences between the collisions with the two species of H_2. Furthermore, it was shown for H_2O–H_2 (Daniel et al. 2011, 2010; Dubernet et al. 2009) that

the effective rate coefficients for $j(H_2) = 2, 3, 4$ are close to the $j(H_2) = 1$ effective rate coefficients. It is probably safe to assume that this is a quasi-general feature. Therefore in the absence of data for $j(H_2)$ greater than 1, thermalized quantum rate coefficients can be estimated using the effective rate coefficients with $j(H_2) = 0, 1$ replacing all others with $j(H_2) = 1$ effective rate coefficients.

2.2.2. Methodologies for collisions with heavy particles

The current heavy-particle BASECOL data is mostly based on collisional calculations performed within the Born-Oppenheimer approximation, which leads to a three-step procedure: calculation of the so-called potential energy surfaces (PES) via ab initio quantum chemistry or empirical methods, representation of the PES by some functional form useful for the dynamical calculations, and finally dynamical calculations. For some specific systems like open-shell radical (OH, NO, CH) in collision with He and H_2 or open-shell atoms (F, Cl) in collision with He and H_2, the collision may induce non adiabatic transitions between different spin-orbit states (Baer 1975; Alexander 1985). In these case, non-Born-Oppenheimer effects have to be taken into account in the dynamical calculations but the general methodology stays the same as for collisions described within the Born-Oppenheimer approximation.

The field of heavy particle molecular collisions underwent intensive development in the 1960s and 1970s. Reviews by Light (1979), Kouri (1979), and Secrest (1979) provide an introduction to quantum close coupling (CC) calculations (Arthurs & Dalgarno 1960) and quantum decoupling approximate methods such as coupled states methods (CS) (McGuire & Kouri 1974; Pack 1974), decoupled l-dominant (DLD) approximation (DePristo & Alexander 1976) and effective Hamiltonian methods (Rabitz 1976). The infinite order sudden (IOS) approximation (Tsien & Pack 1970a,b; Secrest 1975), which combines centrifugal decoupling and the sudden approximation, is often used when other quantum methods are too computationally demanding. These methods have been implemented in the publicly available numerical code MOLSCAT (Hutson & Green 1994; McBane 2004), which is mainly applicable to collisions between closed-shell species ranging from atom-diatom to diatom-asymmetric molecule scattering, and in the codes HIBRIDON (Dagdigian & Alexander 2011)[4] and MOLCOL (Flower et al. 2000), which are designed to treat both open and closed shell systems. It is generally accepted that CC methods are the most accurate ones available, followed by CS, IOS, DLD, and effective Hamiltonian methods. All these methods can calculate state-to-state collisional cross-sections as a function of the relative kinetic energy of the colliding species. Alternatively approaches involving classical or semi-classical approximations are available; the most common approach is the quasi-classical trajectory (QCT) method (Pattengill 1979 and references herein), which solves the classical Hamilton equations using a random (Monte Carlo) sampling of initial conditions combined with a pseudo-quantization of internal energies.

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[4] HIBRIDON is a package of programs for the time-independent quantum treatment of inelastic collisions and photodissociation written by M. H. Alexander, D. E. Manolopoulos, H.-J. Werner, B. Follmeg, Q. Ma, and P. J. Dagdigian, with contributions by P. F. Vohralik, D. Lemoine, G. Corey, R. Gordon, B. Johnson, T. Orlikowski, A. Berning, A. Degli-Esposti, C. Rist, B. Pouilly, G. van der Sanden, M. Yang, F. de Weerd, S. Gregurick, J. Klos and F. Lique. More information and/or a copy of the code can be obtained from the website `http://www2.chem.umd.edu/groups/alexander/hibridon/hib43`.

If the initial and final quantum states of the species are selected, state-to-state collisional cross sections can be computed as for the above quantum methods. The field of molecular collisional for the ISM owns a tribute to the work of Sheldon Green whose entire work can be found in the BASECOL database. Some other relevant references for molecular collision in the ISM can be found in Flower (2007).

The dynamical methods used nowadays have not evolved significantly since the 1970s, as reflected by the methodology information given in BASECOL: see Table A.1 and information sections of BASECOL. Some studies have used a combination of methods, for example, the coupled states method for rotational excitation, and the IOS method for the hyperfine excitation, denoted rCS/hIOS. In other cases, CC is used for low collision energies, and the CS approximation is employed at higher collision energies, denoted CC/CS. If the quantum-mechanical method employed cannot be categorized using the schemes mentioned above, the catch-all notation QM is used.

The increase in computational power has allowed both the treatment of more complex systems and an increase in the accuracy of the dynamical methods used in the calculations. Quantum chemistry calculations have evolved tremendously thanks both to new theoretical developments and to the availability of increasing computer power, making it possible to calculate highly accurate PES. Recently the most popular methods for the closed shell systems included in BASECOL are at the level of the coupled cluster method with single, double, and noniterative triple excitations (CCSD(T)) calculations with large basis sets as implemented in many quantum chemistry packages, see for instance MOLPRO (Werner et al. 2012) or use symmetry-adapted perturbation theory (SAPT) methodologies (Jeziorski et al. 1994; Bukowski et al. 2008). The latter approach has an advantage since the long-range behaviour is fixed at the same level of the theory and on the same basis set (Heijmen et al. 1996). The increase in computer power has also allowed an increase in the number of nuclear geometries spanning the potential energy surface's parameter space, giving an improved description of strongly anisotropic systems and of the long-range part of potential energy surfaces. Nevertheless, for highly anisotropic systems or for systems with many parameters, real difficulties remain with the representation of the highly accurate, calculated ab initio points by functional forms suitable for the dynamical calculations. Poor fits can lead to a loss of accuracy in the functional representation, although there has been some recent progress in this area (Braams & Bowman 2009).

The accuracy of the ab initio potentials can mostly be checked easily by comparing the measured and computed high-resolution spectra, state-to-state cross sections, or rate constants. Some information can also be obtained by comparing the experimental and theoretical differential cross sections, but here the experimental data are usually not state-resolved, and thus are less sensitive to the fine details of the potential. It has been already demonstrated in the 1990s that the ab initio potentials for simple atom-molecule systems like He-CO (Heijmen et al. 1997b) or Ar-CH$_4$ (Heijmen et al. 1999b; Miller et al. 1999) reproduce the experimental high-resolution spectra very well. For some other systems, such Ne-CO (Moszynski et al. 1997) or Ne-C$_2$H$_2$ (Bemish et al. 1998), small scalings were necessary to quantitatively reproduce the experimental data. At the same time, it was shown that the ab initio potentials reproduce the (scarce) data for the state-to-state cross sections and rate constants; see, for instance, Heijmen et al. (1997a) and Heijmen et al. (1999a), respectively. Over the past decade, the complexity of the systems that can be treated by ab initio methods has

increased dramatically; see for instance, Bukowski et al. (2007) and Jankowski et al. (2012), who show the accuracy that can be reached for systems like the water dimer or CO-H_2.

2.2.3. Methodologies for collisions with electrons

The ro-vibrational excitation of molecules by collisions with electrons is a very active field, both experimentally and theoretically. Several theoretical methods and approximations are available, and the interested reader is referred to review papers on electron impact rotational (Itikawa & Mason 2005) and vibrational (Itikawa 2004) excitation. The theoretical procedure differs somewhat from those used for heavy particle collisions since special methods are required to treat the continuum electron. As far as nuclear motion is concerned, the adiabatic-nuclei (AN) approximation, which is similar in spirit to the IOS approximation, has been widely employed to compute rotational and vibrational cross sections (Gianturco & Jain 1986), but is only valid away from resonances where the scattering electron is temporarily trapped to form a quasibound state. The AN approximation has been combined with the R-matrix method to compute inelastic rate coefficients for a variety of astrophysically important molecules, see work by Tennyson and co-workers (Faure & Tennyson 2001; Varambhia et al. 2009) and references therein.

The R-matrix method addresses the electron collision problem by splitting space into two regions: an the inner region where the scattering electron is close to the target, and an outer or long-range region. The wave function in the inner region is expanded in terms of bound and continuum orbitals in a fashion similar to quantum chemistry, whereas a set of close-coupling equations are solved in the outer region. The method has recently been reviewed by Tennyson (2010). For polar species, Born (for neutrals) and Coulomb-Born (for molecular ions) corrections, denoted in Table A.1 as R+Born, are required to account for high partial wave contributions not included in the R-matrix calculations. It is necessary to correct the unphysical behaviour of cross sections at rotational thresholds that are assumed to be degenerate in the AN approximation. For more details, the reader is referred to Varambhia et al. (2009) and references therein. For example, for electron collisions with water, very good agreement is observed with various experimental data once allowance is made for difficulties with measuring forward scattering (Faure et al. 2004b; Zhang et al. 2009). In the case of molecular ions, R+Born calculations have been shown to be accurate, down to very low energies, by comparison with ro-vibrational quantum defect calculations (Faure et al. 2006) and storage ring measurements (Shafir et al. 2009). Alternatively rate coefficients for ro-vibrational excitation of molecular cations by electronic impact can be obtained through the multichannel quantum defect theory (MQDT) as recently done for H_3^+ (Kokoouline et al. 2010).

2.2.4. Fitted and analytic functions of the rate coefficients

BASECOL contains the original published fits to the collisional rate coefficients, when those are available, or provides in-house fits to the published data. The fitting functions as a function of temperature T are provided, and tabulated fitted parameters can be downloaded. In addition a graphical interface allows the user to plot a comparison between the fitted functions and the original data.

The in-house fitting procedure is a part of the quality assessment of the collisional data. Indeed the procedure ensures that detailed balance is respected between interpolation points. As a general rule, it is important to emphasize that these fits have no physical meaning, and are only valid in the temperature range where the data have been calculated; in particular, they should not be used to perform extrapolations. The in-house fitting is provided on request except if authors oppose the idea of providing fits of their data.

2.2.5. Coupling to experimental spectroscopic data as a service to the ISM community

Studies of astrophysical non-LTE media require a combination of collisional and spectroscopic data. Spectroscopic data is provided by databases such as the Cologne Database for Molecular Spectroscopy database (CDMS[5]) (Müller et al. 2001, 2005), the Jet Propulsion Laboratory catalogue (JPL[6]) (Pickett et al. 1998), and the HIgh-resolution TRANsmission molecular absorption database (HITRAN[7]) (Rothman et al. 2009). As a service to the astrophysical community, the SPECTCOL tool (Dubernet et al. 2012; Dubernet & Nenadovic 2011) can be used to associate BASECOL collisional data with spectrocopic data taken from the databases listed above for each BASECOL target. Matched spectroscopic data are available for each collisional system in the sections "Labelling" and 'Einstein". If no spectroscopic data are included, either those will be introduced in the future or no spectroscopic data was found. In the latter case we will try to propose some alternatives based on published spectroscopic data. The last column of Table A.1 indicates which collisional sets are matched with spectroscopic data. Versions of the spectroscopic databases are monitored each week, and updated sets of matched spectroscopic data are generated whenever the spectroscopic data are updated. The different versions of matched queried spectroscopic data are kept for reference and can be retrieved. The collisional data and the matched spectroscopic data can be downloaded either separately in BASECOL format or as a single file with the RADEX format (van der Tak et al. 2007) which is often employed by ISM modellers. We note, however, that RADEX format does not allow for any change of state of the collider and only provides de-excitation rate coefficients. This prevents the user from checking that the calculated rate coefficients satisfy a detailed balance. Therefore our RADEX outputs only keep the initial α and final α' levels ($\alpha > \alpha'$) of the target molecule from $R(\alpha \rightarrow \alpha'; \beta \rightarrow \beta')(T)$ (Eq. (1)), and provide information on the state of the collider. For calculations of state-to-state rate coefficients where the collider is kept in a given state, the state is $\beta = \beta' = 1$. For effective rate coefficients $\hat{R}_\beta(\alpha \rightarrow \alpha')(T)$ (Eq. (3)) the state of the collider indicates that β can be different from 1. For calculations of state-to-state rate coefficients where the internal state of the collider changes, our RADEX outputs keep the state-to-state rate coefficients corresponding to the collider's elastic process alone, i.e. only those transitions corresponding to $\beta = \beta'$, and we indicate the value of β.

2.3. Assessment and recommendation

Column 10 of Table A.1 indicates whether the data are recommended or not, denoted "yes" and "no", respectively. These recommendations are reviewed by the BASECOL team, whose members are the scientific co-authors of this publication. Whenever there is only one available data set, this set is

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[5] http://www.astro.uni-koeln.de/cdms

[6] http://spec.jpl.nasa.gov/

[7] http://www.cfa.harvard.edu/hitran/

recommended except if there are some obvious problems with the calculations. Whenever there are more data sets available, the recommendation is based on the level of theory used in the calculations.

In addition to the level of theory, the quality of the fitting procedure for the PES and the quality of the dynamical calculations is assessed as far as the information provided by the authors allows. For example in CC/CS dynamical calculations, different sources of inaccuracies can emerge: when cross sections are provided on an inadequate grid of collision energies, then the corresponding rate coefficients may be inaccurate, particularly at low and high temperatures; there might be lack of convergence of the basis sets used in the calculation, lack of convergence of the cross sections with respect to total angular momentum, or lack of convergence in the propagation parameters of the differential equation. All these sources of inaccuracies should be carefully checked for different energies and transitions, and in principle an estimate of inaccuracies should be provided by the authors. In addition the authors should provide an assessment of the quality of the potential energy surfaces (see Sect. 2.2.2), as well as comparisons with experimental data when available. The flag "Recommended", indicated on BASECOL interface, is assessed on the basis of the quality information provided by the authors, and the explanation about recommendation is given in the information section associated with each collisional set.

3. Technical characteristics and interoperability through VAMDC

The BASECOL2012 database is freely accessible from http://basecol.vamdc.eu[8] and is currently maintained and mirrored in two geographically distinct locations of Paris Observatory. This ensures long-term maintenance of services and 24-h availability.

Each data set is labeled by a version number with the date of "publication" or "modification" of the data set on the BASECOL2012 website. A modification would correspond to errors found in the datasets after the date of BASECOL publication. Modification of the data description does not lead to a new version of the data set. The history of version is given at the bottom of each data set main webpage. The version number, together with the corresponding date of publication or modification, is indicated in the data set's file name, which can be downloaded in ASCII. The version of external spectroscopic data follows the version procedure of the original database.

BASECOL2012 is interoperable within the Virtual Atomic and Molecular Data Center (VAMDC) (Dubernet et al. 2010; Endres et al. 2011; Rixon et al. 2011); i.e., it is interoperable with the current 24 atomic and molecular databases registered within VAMDC and can be queried by any client that implements the VAMDC standards[9].

In particular, BASECOL2012 is accessible from the VAMDC portal[10] and from the SPECTCOL tool (Dubernet et al. 2012; Dubernet & Nenadovic 2011)[11]; that allow a user to mix any sets of BASECOL collisional rate coefficients with any sets of spectroscopic data. The SPECTCOL tool evolves with user requirements, and the last version includes the possibilities of scaling the collisional rate coefficients, output of the data in the RADEX format (van der Tak et al. 2007) and of discarding quantum numbers when matching BASECOL energy levels with external databases energy levels. This last feature is very useful because the XSAMS schema[12] allows redundant information to be transferred.

4. Perspectives

A well-maintained database is an evolving product, and some new features are foreseen. The "Publication" section will be upgraded with regular notes concerning new data and/or evaluation. Once the VAMDC standards are more stable, the BASECOL energy levels (section "Labelling Energy levels"), rate coefficients (section "Rate Coefficients"), and the combined "Radiation/Collision" data will be emitted in XSAMS format for download. We intend to provide a password-protected administrative interface enabling scientists to upload their most recent results themselves. As a service to the astrophysics community, we also intend to create some in-house combined collisional sets that will include extrapolations in order to cover the full range of temperatures and transitions necessary for the astrophysical applications.

Appendix A: Comments on some collisional systems

A.1. Excitation of H_2

In some CC or CS calculations, some collisional sets have been obtained with rotational or rovibrational basis sets that are missing a few energy levels, because the basis set cuts were performed using the principal rotational quantum number instead of using a cut at a given energy. This is the case for H_2 calculations and BASECOL has replaced the corresponding missing collisional transitions by a value of zero for the rate coefficients for the whole range of temperature. For collision identifier (ID) 24 and 26 (see Col. 1 of Table A.1), the rate coefficients have not been calculated for transitions involving level 24 of ortho-H_2, (i.e. $v = 1$, $j = 11$), but are available for transitions involving level 25 ($v = 3$, $j = 7$). Therefore all rate coefficients involving level 24 are set to zero. For ID = 25, 27, 31, the rate coefficients have not been calculated for transitions involving level 27 of para-H_2, (i.e. $v = 1$, $j = 14$), but are available for transitions involving level 28 ($v = 3$, $j = 8$). Therefore all rate coefficients involving level 27 are set to zero. For ID = 28 the rate coefficients have not been calculated for transitions involving levels 18, 20 of ortho-H_2, (i.e. $v = 3$, $j = 1$; $v = 3$, $j = 3$). Therefore all rate coefficients involving levels 18, 20 are set to zero.

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8 Equivalent to http://basecol.vamdc.org, http://basecol.obspm.fr, http://basecol.obs-besancon.fr

9 http://www.vamdc.eu/standards

10 www.vamdc.eu/portal

11 www.vamdc.eu/software

12 http://vamdc.eu/standards

A.2. Excitation of CH$_3$OH

Quantum numbers and symmetries used to label the energy levels of methanol have not been agreed on yet within VAMDC and therefore the notation of Rabli & Flower (2010a,b, 2011) are used in BASECOL. This notation might evolve in the future.

A.3. Excitation of H$_3$O$^+$ by electrons

The collision sets of o/p-H$_3$O$^+$ (Faure & Tennyson 2003) have incomplete transitions because the authors considered only the $K = 0$ and $K = 1$ ladders. The authors expect to complete the original calculations by adding the $K > 1$ levels and extending the temperatures down to 10 K.

A.4. Excitation of H$_3^+$ by electrons

The recommended sets of o/p-H$_3^+$ by electrons (Kokoouline et al. 2010) use a complete set of energy levels up to the 7th rotational level for o-H$_3^+$ and up to the 13th rotational level for p-H$_3^+$. Nevertheless, the collisional sets miss some transitions between energy levels. The missing collisional rate coefficients can be set equal to zero as the missing rate coefficients are typically three orders of magnitude smaller than the given collisional data.

A.5. Excitation of o–H$_2$O / p–H$_2$O by electrons

The collision rotational sets of o/p-H$_2$O-electron (Faure et al. 2004a) are only complete among the first 14th rotational levels. The user is advised to use the ro-vibrational collisional sets of Faure & Josselin (2008) for transitions from levels above the 14th rotational level and for temperature above 200 K.

A.6. Excitation of SiC$_2$ and c-C$_3$H$_2$

The work of Green et al. (1987) on excitation of c-C$_3$H$_2$ by He has been used by Chandra & Kegel (2000) to provide state-to-state rate coefficients between the 47 lowest ortho levels and the 48 lowest para levels of c-C$_3$H$_2$ colliding with H$_2$, for $T = 30$, 60, 90, 120 K. In the same paper, the work of Palma & Green (1987) on excitation of SiC$_2$ by He has been used to provide state-to-state rate coefficients among the lowest 40 energy levels of SiC$_2$ colliding with H$_2$ and for temperature $T = 25$, 50, 75, 100, 125 K. In BASECOL the calculations have been redone using the same ingredients as Chandra & Kegel (2000), and we found that Chandra & Kegel (2000) do not provide rate coefficients for collisions of c-C$_3$H$_2$ and SiC$_2$ with H$_2$, as the title of their paper indicates, but instead collisions with He. The LAMDA database Schöier et al. (2005) gives the wrong indication on this matter.

A.7. Excitation of o–H$_2$O / p–H$_2$O by He, H$_2$ and recommendation

Owing to its importance in astrophysical studies, the calculation of collisional rate coefficients for the water molecule have been refined through the past decades, and many sets are available for this molecule. The first set that was available to the astrophysicists considered He as a collisional partner (Green et al. 1993). This set can still be considered as a reference, but only if collisions with He are considered explicitly in the modelling. This set of rates must not be used to emulate collisions with H$_2$ by using an ad hoc scaling factor. The specific consideration of H$_2$ as a collisional partner was first considered by Phillips et al. (1996). However, these early calculations, which covered a reduced number of temperatures and water energy levels, have been outclassed due to the calculation of a most accurate PES (Faure et al. 2005; Valiron et al. 2008), which has been used to calculate collisional rate coefficients with the QCT method (Faure et al. 2007b) and with the quantum CC approach (Dubernet et al. 2009; Daniel et al. 2010, 2011). This latter set is the most accurate and outclass the QCT set. We note that the highest temperature considered in the quantum set is 1500 K while the QCT calculation extend to 2000 K. These highest temperatures can be of interest in the study of the envelopes of AGB stars (Royer et al. 2010; Neufeld et al. 2011) or to study shock regions (Nisini et al. 2010; Flower & Pineau des Forêts 2012). For the range of temperature 1500–2000 K, we still recommend using the quantum set rather than the QCT set, by extrapolating the collisional rate coefficients. Indeed, the comparison of the QCT and quantum rate coefficients made in Daniel et al. (2012) showed that even at high temperature, the QCT rate coefficients and quantum thermalized rate coefficients can predict intensities that differ by up to a factor 3, an error which can be directly linked to the difference in the magnitude of the rate coefficients which is also typically of a factor 3. Extrapolating the quantum rate coefficients should thus be more reliable.

Additionally, Faure & Josselin (2008) provide ro–vibrational rate coefficients for the first five vibrational levels of both o-H$_2$O and p–H$_2$O and for the range of temperature 200–5000 K. Due to the high temperatures considered by this set, it is still recommended when the ro–vibrational excitation has to be considered. However, for the range of temperature covered by the quantum CC calculations in $(v1, v2, v3) = (0, 0, 0)$, i.e. $Tk = 20-1500$ K, this set must not be used and the quantum CC calculations should be used instead. Indeed, for the rotational transitions among a given vibrational state, the rate coefficients of the Faure & Josselin (2008) set are taken to be equal to the QCT rates of Faure et al. (2007b) in $(v1, v2, v3) = (0, 0, 0)$. These rates can be directly replaced by the quantum CC rate coefficients. For the collisional transitions between different vibrational states, the Faure & Josselin (2008) rates still correspond to the QCT rate coefficients of Faure et al. (2007b) but are scaled by a factor $P(v - v')$ which has been determined experimentally. In this case, we recommend to use the quantum CC rate coefficients and multiply these rates by the factor $P(v - v')$ provided by Faure & Josselin (2008).

Table A.1. Summary of atomic and molecular collisional data in BASECOL2012.

Id	Target	Collider	Levels	Temperature (K)	Method	Method's Ref	PES Ref	Year	Recom	Fit	Matched
101	C	H	f3	5–1000	CC	2	75	2007	yes	y	n
116	C	H	f3	4–1000	CC	1	74	1977	no	y	n
106	C	o-H$_2$	f3	10–1200	CC	3	3	1991	yes	y	n
105	C	p-H$_2$	f3	10–1200	CC	3	3	1991	yes	y	n
104	C	He	f3	10–150	CC	4	4	1991	yes	y	n
102	C$^+$	H	f2	20–2000	CC	5	76	2005	yes	y	n
145	C$_3$	He	r6	5–15	CC	6	6	2008	yes	n	n
214	C$_4$	He	r20f30	1–50	CC	122	122	2010	yes	n	n
201	C$_2$H	He	h34	5–100	CC+recoup	104	104	2012	yes	n	n
192	CH$^+$	He	r11	20–200	CC	7	7	2008	no	n	y

Notes. The "Method" notations CC, CS, IOS, QCT are explained in the text, "R" stands for R-matrix calculations, "born" stands for Born and Born-Coulomb approximations, VCC-IOS means that vibration is treated with CC and rotation with IOS, hIOS means that the hyperfine transitions are treated with IOS, "approx" means that some additional approximation has been performed, "recoupl" means that a recoupling technique for T or S matrices has been used to obtain the hyperfine cross sections. The different columns provide the following information: (1:) ID by which the collisional system can be found directly in the database, (2:) the available atomic or molecular target, (3:) the perturbing collider, (4:) the rovibrational levels for which rate coefficients are available: the symbols r, f, v, rv and h are used to denote rotational, fine, vibrational, ro-vibrational and hyperfine transitions respectively (for example, "r7" means that rate coefficients are available for the 7 lowest rotational levels), (5:) temperature range for which the rates have been calculated, (6:) method employed to treat the collision dynamics, (7,8:) references to the papers describing the calculations and the potential energy surfaces calculations respectively, (10:) whether the set is recommended, (11:) whether fitting coefficients are available, and the last column indicates whether the collisional set is matched with spectroscopic data (see Sect. 2.2.5).

References. (1) Launay & Roueff (1977). (2) Abrahamsson et al. (2007). (3) Schröder et al. (1991). (4) Staemmler & Flower (1991). (5) Barinovs et al. (2005). (6) Ben Abdallah et al. (2008). (7) Hammami et al. (2008a). (8) Lim et al. (1999). (9) Chandra & Kegel (2000). (10) Balakrishnan et al. (2002). (11) Wernli et al. (2006). (12) Flower (2001a). (13) Sarpal & Tennyson (1993). (14) Cecchi-Pestellini et al. (2002). (15) Faure & Tennyson (2001). (16) Green & Chapman (1978). (17) Turner et al. (1992). (18) Lique et al. (2006b). (19) Lique & Spielfiedel (2007). (20) Forrey et al. (1997). (21) Flower & Roueff (1998a). (22) Flower & Roueff (1999b). (23) Flower & Roueff (1998b). (24) Flower et al. (1998). (25) Faure & Tennyson (2003). (26) Green (1991). (27) Phillips et al. (1996). (28) Faure et al. (2007a). (29) Dubernet et al. (2009). (30) Faure & Josselin (2008). (31) Green et al. (1993). (32) Faure et al. (2004a). (33) Wernli et al. (2007a,b). (34) Neufeld & Green (1994). (35) Green & Thaddeus (1974). (36) Monteiro & Stutzki (1986). (37) Faure et al. (2007b). (38) Hammami et al. (2008). (39) Hammami et al. (2008b). (40) Monteiro (1984). (41) Roueff & Flower (1999). (42) Flower (1999a). (43) Flower (1999b). (44) Roueff & Zeippen (1999). (45) Green (1989). (46) Reese et al. (2005). (47) Hammami et al. (2007). (48) Rabadan et al. (1998). (49) Green (1975). (50) Daniel et al. (2005). (51) Machin & Roueff (2007). (52) Machin & Roueff (2006). (53) Danby et al. (1986). (54) Danby et al. (1988). (55) Machin & Roueff (2005). (56) Danby et al. (1987). (57) Jaquet et al. (1992). (58) Flower (2001b). (59) Toboła et al. (2007). (60) Nkem et al. (2009). (61) Kłos et al. (2008). (62) Dayou & Balança (2006). (63) Varambhia et al. (2009). (64) Kłos & Lique (2008). (65) Vincent et al. (2007). (66) Toboła et al. (2008). (67) Green (1994). (68) Lique et al. (2007). (69) Lique et al. (2006c). (70) Lique et al. (2006a). (71) Lique et al. (2005). (72) Green (1995). (73) Toboła et al. (2011). (74) Yau & Dalgarno (1976). (75) Kalemos et al. (1999). (76) Barinovs & van Hemert (2004). (77) Hammami et al. (2009). (78) Turpin et al. (2010). (79) Green et al. (1987). (80) Keller et al. (1996). (81) Jankowski & Szalewicz (1998). (82) Jankowski & Szalewicz (1998). (83) Heijmen et al. (1997c). (84) Boothroyd et al. (1996). (85) Schwenke (1988). (86) Muchnick & Russek (1994). (87) Garrison & Lester (1975). (88) Phillips et al. (1994). (89) Valiron et al. (2008). (90) Maluendes et al. (1992). (91) Monteiro (1985). (92) Palma et al. (1988). (93) Stoecklin et al. (2003). (94) Daniel et al. (2004). (95) Hodges & Wheatley (2001). (96) Parlant & Yarkony (1999). (97) Higgins & Klemperer (1999). (98) Palma & Green (1987). (99) Palma (1987). (100) Kłos et al. (2000). (101) Maret et al. (2009). (102) Troscompt et al. (2009). (103) Cybulski et al. (2005). (104) Spielfiedel et al. (2012). (105) Cernicharo et al. (2011). (106) Spielfiedel et al. (2009). (107) Dumouchel et al. (2010). (108) Sarrasin et al. (2010). (109) Toczyłowski et al. (2001). (110) Ben Abdallah et al. (2012). (111) Faure et al. (2012). (112) Lique (2010). (113) Groenenboom & Struniewicz (2000). (114) Kłos et al. (2009). (115) Cybulski et al. (2000). (116) Kłos et al. (2007). (117) Lee et al. (2000). (118) Kłos & Lique (2011). (119) Lique et al. (2010b). (120) Lique & Kłos (2011). (121) Kalugina et al. (2012). (122) Lique et al. (2010a). (123) Yang et al. (2010). (124) Flower & Roueff (1999a). (125) Rabli & Flower (2010b). (126) Pottage et al. (2002). (127) Rabli & Flower (2010a). (128) Pottage et al. (2004). (129) Rabli & Flower (2011). (130) Dumouchel et al. (2011). (131) Kokoouline et al. (2010).

Table A.1. continued.

Id	Target	Collider	Levels	Temperature (K)	Method	Method's Ref	PES Ref	Year	Recom	Fit	Matched
146	CH+	He	r11	20–2000	CC	77	7	2009	yes	n	y
191	CH+	He	r6	1–200	CC	78	78	2010	yes	n	y
160	CH+	e	r8	100–15 000	R	8	8	1999	yes	y	y
224	A-CH3OH	He	r256, $ut = 0$	10–200	CS	125	126	2010	yes	n	n
226	A-CH3OH	He	r256, $ut = 1$	10–200	CS	125	126	2010	yes	n	n
229	A-CH3OH	He	r256, $ut = 2$	10–200	CS	125	126	2010	yes	n	n
225	E-CH3OH	He	r256, $ut = 0$	10–200	CS	125	126	2010	yes	n	n
227	E-CH3OH	He	r256, $ut = 1$	10–200	CS	125	126	2010	yes	n	n
228	E-CH3OH	He	r256, $ut = 2$	10–200	CS	125	126	2010	yes	n	n
230	A-CH3OH	p-H₂	r256, $ut = 0$	10–200	CS	127	128	2010	yes	n	n
231	A-CH3OH	p-H₂	r256, $ut = 1$	10–200	CS	127	128	2010	yes	n	n
232	A-CH3OH	p-H₂	r256, $ut = 2$	10–200	CS	127	128	2010	yes	n	n
233	E-CH3OH	p-H₂	r256, $ut = 0$	10–200	CS	127	128	2010	yes	n	n
234	E-CH3OH	p-H₂	r256, $ut = 1$	10–200	CS	127	128	2010	yes	n	n
235	E-CH3OH	p-H₂	r256, $ut = 2$	10–200	CS	127	128	2010	yes	n	n
222	A-CH3OH	He	rvt150	10–400	CS	129	126	2011	yes	n	n
223	E-CH3OH	He	rvt150	10–400	CS	129	126	2011	yes	n	n
46	o c-C₃H₂	He	r47	30–120	IOS	9,79	79	2000	yes	y	y
47	p c-C₃H₂	He	r48	30–120	IOS	9,79	79	2000	yes	y	y
210	CN⁻	p-H₂	r11	5–100	CS	118	118	2011	yes	n	y
211	CN⁻	o-H₂	r11	5–100	CS	118	118	2011	yes	n	y
209	CN	He	r21f41	5–350	CC	119	119	2010	yes	n	n
212	CN	He	r13h73	5–30	CC+recoupl	120	119	2011	yes	n	n
213	CN	p-H₂	r6h37	5–100	CC+recoupl	121	121	2012	yes	n	n
48	CO	H	r8	5–100	CC	10	80	2002	yes	y	y
60	CO	H	r17	100–3000	CC	10	80	2002	yes	y	y
49	CO	H	v5	100–3000	IOS	10	80	2002	yes	y	n
218	CO	o-H₂	r41	1–3000	CC/CS	123	81	2010	yes	y	y
219	CO	p-H₂	r41	1–3000	CC/CS	123	81	2010	yes	y	y
97	CO	o-H₂	r6	5–70	CC/CS	11	81	2006	no	y	y
98	CO	p-H₂	r6	5–70	CC/CS	11	81	2006	no	y	y
33	CO	o-H₂	r20	5–400	CC	12	82	2001	no	y	y
34	CO	p-H₂	r29	5–400	CC	12	82	2001	no	y	y
50	CO	He	r15	5–500	CC	14	83	2002	yes	y	y
51	CO	He	v7	500–5000	IOS	14	83	2002	yes	n	y
161	CO+	e	r5	100–10 000	R	15	15	2001	no	y	n
61	CS	p-H₂	r13	10–100	CC/CS	16	16	1978	yes	y	y
10	CS	p-H₂	r21	20–300	CC/CS	17	16	1992	yes	y	n
90	CS	He	r31	10–300	CC	18	18	2006	yes	y	n
121	CS	He	v3 (r38 in each v)	300–1500	VCC-IOS	19	19	2007	yes	n	y
54	o-H₂	H	r3	100–1000	CC	20	84	1997	yes	y	n
53	p-H₂	H	r3	100–1000	CC	20	84	1997	yes	y	n
26	o-H₂	H	v1r8,v2r7,v3r5,v4r4 (up to l25)	100–6000	CC	21	84	1998	yes	y	n
27	p-H₂	H	v1r9,v2r7,v3r6,v4r5 (up to l28)	100–6000	CC	21	84	1998	yes	y	n
28	o-H₂	o-H₂	v1r7,v2r6,v3r4 (up to l22)	100–6000	CC	21	85	1999	yes	y	n
30	p-H₂	o-H₂	v1r8,v2r6,v3r5 (up to l19)	100–6000	CC	21	85	1999	yes	y	n
29	o-H₂	p-H₂	v1r13,v2r11,v3r5 (up to l24)	100–6000	CC	23	85	1998	yes	y	n
31	p-H₂	p-H₂	v1r9,v2r7,v3r6,v4r5 (up to l28)	100–6000	CC	23	85	1998	yes	y	n

Table A.1. continued.

Id	Target	Collider	Levels	Temperature (K)	Method	Method's Ref	PES Ref	Year	Recom	Fit	Matched
24	o-H_2	He	v1r8,v2r7,v3r5,v4r4 (up to 125)	100–6000	CC	24	86	1998	yes	y	n
25	p-H_2	He	v1r9,v2r7,v3r6,v4r5 (up to 128)	100–6000	CC	24	86	1998	yes	y	n
165	o-H_2^+	e	r2	100–10 000	R	15	15	2001	yes	y	n
166	p-H_2^+	e	r2	100–10 000	R	15	15	2001	yes	y	n
178	H_2^+	e	v3	100–20 000	R	13	13	1993	yes	y	n
168	o-H_3^+	e	r2	100–10 000	R	25	25	2003	no	y	n
167	p-H_3^+	e	r4	100–10 000	R	25	25	2003	no	n	n
240	o-H_3^+	e	r7	5–2000	MQDT	131	131	2010	yes	n	n
241	p-H_3^+	e	r13	5–2000	MQDT	131	131	2010	yes	y	n
170	o-H_3O^+	e	r4	100–10 000	R	25	25	2003	yes	y	n
169	p-H_3O^+	e	r8	100–10 000	R	25	25	2003	yes	y	n
18	o-H_2CO	He	r41	10–300	CC/CS	25	87	1991	yes	y	y
17	p-H_2CO	He	r40	10–300	CC/CS	25	87	1991	yes	y	y
198	o-H_2CO	p-H_2	r10	5–100	CC/CS	102	102	2009	yes	y	y
199	o-H_2CO	o-H_2	r10	5–100	CC/CS	102	102	2009	yes	y	n
41	o-H_2O	o-H_2	r5	20–140	CC/CS	27	88	1996	no	y	y
42	o-H_2O	p-H_2	r5	20–140	CC/CS	27	88	1996	no	y	y
43	p-H_2O	o-H_2	r5	20–140	CC/CS	27	88	1996	no	y	y
44	p-H_2O	p-H_2	r5	20–140	CC/CS	27	88	1996	no	y	y
190	o-H_2O	o-H_2	r45	20–2000	QCT	28	89	2007	no	y	n
189	o-H_2O	p-H_2	r45	20–2000	QCT	28	89	2007	no	y	n
188	p-H_2O	o-H_2	r45	20–2000	QCT	28	89	2007	no	y	n
187	p-H_2O	p-H_2	r45	20–2000	QCT	28	89	2007	no	y	n
127	o-H_2O	p-H_2	r45	5–1500	CC	29	89	2009	yes	y	y
193	o-H_2O	o-H_2	r45	5–1500	CC	91	89	2011	yes	y	y
194	p-H_2O	p-H_2	r45	5–1500	CC	91	89	2011	yes	y	y
195	o-H_2O	o-H_2	r45	5–1500	CC	90, 91	89	2010, 2011	yes	y	y
4	o-H_2O	He	r45	20–2000	CC/CS	31	90	1993	yes	y	y
22	p-H_2O	He	r45	20–2000	CC/CS	31	90	1993	yes	y	y
134	o-H_2O	e	r14	100–8000	R	32	32	2004	yes	y	y
128	p-H_2O	e	r14	100–8000	R	32	32	2004	yes	y	y
182	o-H_2O	H_2	rv411	200–5000	QCT + approx	30	89	2008	yes	n	n
181	p-H_2O	H_2	rv411	200–5000	QCT + approx	30	89	2008	yes	n	n
184	o-H_2O	e	rv411	200–5000	R + approx	30	32	2008	yes	n	n
183	p-H_2O	e	rv411	200–5000	R + approx	30	32	2008	yes	n	n
140	o-D_2O	e	r18	100–8000	R	32	32	2004	yes	y	n
135	p-D_2O	e	r18	100–8000	R	32	32	2004	yes	y	n
207	o-D_2O	p-H_2	r6	5–100	CC	111	89	2012	yes	n	n
215	p-D_2O	p-H_2	r6	5–100	CC	111	89	2012	yes	n	n
216	HDO	p-H_2	r30	5–300	CC/CS	111	89	2012	yes	n	n
217	HDO	o-H_2	r30	5–300	CC/CS	111	89	2012	yes	n	n
36	HC_3N	He	r21	10–80	QCT/IOS	16	16	1978	no	n	n
175	HC_3N	He	r11	10–20	CC	33	33	2007	yes	n	y
174	HC_3N	p-H_2	r51	10–100	CC/CS/QCT	33	33	2007	yes ?	y	y
13	HCl	He	r8	10–300	CC/CS	34	34	1994	yes	n	y
14	HCl	He	h28	10–300	CC/CS/hIOS	34	34	1994	yes	n	y
62	HCN	He	r8	5–100	CC	35	35	1974	no	y	y

Table A.1. continued.

Id	Target	Collider	Levels	Temperature (K)	Method	Method's Ref	PES Ref	Year	Recom	Fit	Matched
202	HCN	He	r26	5–500	CC	107, 108	109	2010	yes	y	y
203	HNC	He	r26	5–500	CC	107, 108	108	2010	yes	y	y
238	HNC	p-H2	r11	5–100	CC	130	130	2011	yes	y	y
239	HNC	o-H2	r11	5–100	CC	130	130	2011	yes	y	y
92	HCN	He	r4h13	10–30	CC	36	35	1986	no	y	y
204	HCN	p-H2	r10h31	5–100	CC+recoup	110	110	2012	yes	n	n
147	HCN	e	r9	5–2000	R+Born	37	37	2007	yes	y	y
153	HCN	e	r3h10	10–100–1000	R+Born +hIOS	37	37	2007	yes	n	n
150	HNC	e	r9	5–2000	R+Born	37	37	2007	yes	y	y
155	HNC	e	r3h10	10–1000	R+Born+hIOS	37	37	2007	yes	y	n
157	DCN	e	r9	5–2000	R+Born	37	37	2007	yes	y	y
154	DCN	e	r3h10	10–100–1000	R+Born+hIOS	37	37	2007	yes	y	n
151	DNC	e	r9	5–2000	R+Born	37	37	2007	yes	y	y
154	DNC	e	r3h10	10–100–1000	R+Born+hIOS	37	37	2007	yes	y	n
11	HCO$^+$	p-H$_2$	r21	5–390	CC	43	91	1999	yes	y	y
163	HCO$^+$	e	r3	100–10 000	R+Born	15	15	2001	yes	y	y
144	HCP	p-H$_2$	r11	10–70	CC	38	38	2008	yes	n	y
143	HCP	He	r16	20–200	CC	39	39	2008	yes	n	y
19	HCS$^+$	He	r11	10–60	CC/CS	40	40	1984	yes	n	y
70	HD	H	r9	100–2000	CC	41	84	1999	yes	n	n
71	HD	H	v2r9	100–2080	CC	124	84	1999	yes	n	n
72	HD	He	r10	80–1000	CC	44	86	1999	yes	n	n
73	HD	o-H$_2$	r9	50–500	CC	42	85	1999	yes	y	n
74	HD	p-H$_2$	r9	50–500	CC	42	85	1999	yes	y	n
75	HD	o-H$_2$	v2r9	100–2080	CC	124	85	1999	yes	n	n
76	HD	p-H$_2$	v2r9	100–2080	CC	124	85	1999	yes	n	n
21	HDO	He	r34	50–500	CC/CS	45	92	1989	yes	y	y
141	HDO	e	r36 (a-type)	100–8000	R	32	32	2004	yes	y	n
142	HDO	e	r36 (b-type)	100–8000	R	32	32	2004	yes	y	n
63	HF	He	r10	0.1–300	CC	46	93	2005	yes	n	y
176	HeH$^+$	e	r3	100–20 000	R	48	48	1998	yes	y	y
177	HeH$^+$	e	v3	100–20 000	R	48	48	1998	yes	y	n
122	HOCO+	He	r25	10–30	CS	47	47	2007	yes	n	y
208	NH	He	r8f25	5– 350	CC	73	103	2011	yes	y	y
91	N$_2$H$^+$	He	r7	5–40	CC	49	49	1975	no	y	y
82	N$_2$H$^+$	He	r7	5–50	CC	50	94	2005	yes	n	y
69	N$_2$H$^+$	He	r7h55	5–50	CC+S-recoup	50	94	2005	yes	n	y
125	o-ND$_2$H	He	r9	5–100	CS	51	51, 95	2007	yes	n	y
126	p-ND$_2$H	He	r9	5–100	CS	yes	51, 95	2007	yes	n	y
124	o-NH$_2$D	He	r9	5–100	CS	52	52, 95	2006	yes	n	y
123	p-NH$_2$D	He	r9	5–100	CS	52	52, 95	2006	yes	n	n
85	o-NH$_3$	p-H$_2$	r9	15–300	CC	53	53	1986	no	n	y
87	p-NH$_3$	p-H$_2$	r16	15–300	CC	56	53	1987	no	y	y
88	o-NH$_3$	p-H$_2$	r17	15–300	CC	54	53	1988	yes	n	y
89	p-NH$_3$	p-H$_2$	r24	15–300	CC	54	53	1988	yes	n	y
196	o-NH$_3$	p-H$_2$	r6	5–100	CC	101	101	2009	yes	n	n
197	p-NH$_3$	p-H$_2$	r16	5–100	CC	101	101	2009	yes	n	n

Table A.1. continued.

Id	Target	Collider	Levels	Temperature (K)	Method	Method's Ref	PES Ref	Year	Recom	Fit	Matched
83	o-NH$_3$	He	r22	5–300	CC	55	95	2005	yes	n	y
84	p-NH$_3$	He	r16	5–300	CC	55	95	2005	yes	y	y
185	NO	He	f98	10–500	CS	61	100	2008	yes	n	n
164	NO$^+$	e	r5	100–5000	R	15	15	2001	yes	y	y
117	O	H	f3	50–1000	CC	1	1	1977	no	y	n
107	O	H	f3	50–1000	CC	2	96	2007	yes	y	n
109	O	o-H$_2$	f3	20–1500	CC	57	57	1992	yes	y	n
108	O	p-H$_2$	f3	20–1500	CC	57	57	1992	yes	y	n
35	OCS	p-H$_2$	r13	10–100	CS	16	16	1978	yes	y	y
12	OCS	He	r27	10–150	CC	58	97	2001	yes	y	y
206	OH	He	f46	5–350	CC	116	117	2007	yes	n	n
205	O$_2$	He	r23f36	5–350	CC	112	113	2010	yes	n	n
118	PN	He	r31	5–300	CC/CS	59	59	2007	yes	n	n
103	Si$^+$	H	f2	20–2000	CC	5	5	2005	yes	y	n
179	SiH$^+$	He	r11	5–200	CC	60	60	2009	yes	n	n
45	o-SiC$_2$	He	r40	25–125	IOS	9,98	98	2000	no	y	y
23	SiO	p-H$_2$	r21	20–300	CS	17	17	1992	yes	y	y
100	SiO	p-H$_2$	r27	10–300	CC	62	62	2006	yes	y	y
95	SiO	He	r27	10–300	CC	62	62	2006	yes	y	y
186	SiO	e	r41	5–5000	R	63	63	2009	yes	y	y
172	SiS	o-H$_2$	r41	5–300	CS	64	64	2008	yes	y	y
171	SiS	p-H$_2$	r41	5–300	CS	64	64	2008	yes	y	y
119	SiS	He	r26	5–200	CC	65	65	2007	yes	y	y
173	SiS	He	v5r100	100–1500	VCC+IOS	66	66	2008	yes	n	n
200	SH	He	f58	5–350	CC	114	115	2009	yes	n	y
32	SO	p-H$_2$	r24f70	50–350	rCS+fIOS	67	67	1994	no	n	n
180	SO	p-H$_2$	r31	5–50	CC	68	68	2007	yes	n	n
96	SO	He	rv236	300–800	VCC–IOS	69	69	2006	yes	n	y
81	SO	He	f91	60–300	CC/IOS	70	71	2006	yes	y	y
77	SO	He	f31	5–50	CC	71	71	2005	yes	n	y
20	SO$_2$	He	r50	25–125	IOS	72	99	1995	no	y	y
220	SO$_2$	p-H$_2$	r31	5–30	CC	105	106	2011	yes	n	n
221	SO$_2$	o-H$_2$	r31	5–30	CC	105	106	2011	yes	n	n

References

Abrahamsson, E., Krems, R. V., & Dalgarno, A. 2007, ApJ, 654, 1171
Alexander, M. 1985, Chem. Phys., 92, 337
Arthurs, A. M., & Dalgarno, A. 1960, Proc. R. Soc. A, 256, 540
Baer, M. 1975, Chem. Phys. Lett., 35, 112
Balakrishnan, N., Yan, M., & Dalgarno, A. 2002, ApJ, 568, 443
Barinovs, G., & van Hemert, M. 2004, Chem. Phys. Lett., 399, 406
Barinovs, Ğ., van Hemert, M. C., Krems, R., & Dalgarno, A. 2005, ApJ, 620, 537
Bemish, R., Oudejans, L., Miller, R., et al. 1998, J. Chem. Phys., 109, 8968
Ben Abdallah, D., Hammami, K., Najar, F., et al. 2008, ApJ, 686, 379
Ben Abdallah, D., Najar, F., Jaidane, N., Dumouchel, F., & Lique, F. 2012, MNRAS, 419, 2441
Bergin, E. A., Phillips, T. G., Comito, C., et al. 2010, A&A, 521, L20
Boothroyd, A. I., Keogh, W. J., Martin, P. G., & Peterson, M. R. 1996, J. Chem. Phys., 104, 7139
Braams, B. J., & Bowman, J. M. 2009, Int. Rev. Phys. Chem., 28, 577
Bukowski, R., Szalewicz, K., Groenenboom, G., & Van der Avoird, A. 2007, Science, 315, 1249
Bukowski, R., Cencek, W., Jankowski, P., et al. 2008, SAPT2008: An Ab Initio Program for Many-Body Symmetry-Adapted Perturbation Theory Calculations of Intermolecular Interaction Energies (University of Delaware and University of Warsaw)
Caux, E., Kahane, C., Castets, A., et al. 2011, A&A, 532, A23
Ceccarelli, C., Bacmann, A., Boogert, A., et al. 2010, A&A, 521, L22
Cecchi-Pestellini, C., Bodo, E., Balakrishnan, N., & Dalgarno, A. 2002, ApJ, 571, 1015
Cernicharo, J., Spielfiedel, A., Balança, C., et al. 2011, A&A, 531, A103
Chandra, S., & Kegel, W. H. 2000, A&AS, 142, 113
Cybulski, S. M., Toczylowski, R. R., Lee, H.-S., & McCoy, A. B. 2000, J. Chem. Phys., 113, 9549
Cybulski, S. M., Krems, R. V., Sadeghpour, H. R., et al. 2005, J. Chem. Phys., 122, 094307
Dagdigian, P., & Alexander, M. H. 2011, J. Chem. Phys., 135, 064306
Danby, G., Flower, D. R., Kochanski, E., Kurdi, L., & Valiron, P. 1986, J. Phys. B At. Mol. Opt. Phys., 19, 2891
Danby, G., Flower, D. R., Valiron, P., Kochanski, E., & Kurdi, L. 1987, J. Phys. B At. Mol. Opt. Phys., 20, 1039
Danby, G., Flower, D. R., Valiron, P., Schilke, P., & Walmsley, C. M. 1988, MNRAS, 235, 229
Daniel, F., Dubernet, M.-L., & Meuwly, M. 2004, J. Chem. Phys., 121, 4540
Daniel, F., Dubernet, M.-L., Meuwly, M., Cernicharo, J., & Pagani, L. 2005, MNRAS, 363, 1083
Daniel, F., Dubernet, M.-L., Pacaud, F., & Grosjean, A. 2010, A&A, 517, A13
Daniel, F., Dubernet, M.-L., & Grosjean, A. 2011, A&A, 536, A76
Daniel, F., Goicoechea, J. R., Cernicharo, J., Dubernet, M.-L., & Faure, A. 2012, A&A, 547, A81
Dayou, F., & Balança, C. 2006, A&A, 459, 297
de Graauw, T., Helmich, F. P., Phillips, T. G., et al. 2010, A&A, 518, L6
DePristo, A. E., & Alexander, M. H. 1976, J. Chem. Phys., 64, 3009
Drouin, B., & Wiesenfeld, L. 2012, Phys. Rev. A, 86, 2705
Drouin, B. J., Pearson, J. C., & Dick, M. J. 2010, Phys. Rev. A, 82, 6704
Dubernet, M.-L., & Nenadovic, L. 2011, in Astrophysics Source Code Library, ascl:1111.005
Dubernet, M. L., Grosjean, A., Flower, D., et al. 2006, J. Plasma Res. Ser., 7, 356
Dubernet, M.-L., Daniel, F., Grosjean, A., & Lin, C. Y. 2009, A&A, 497, 911
Dubernet, M. L., Boudon, V., Culhane, J. L., et al. 2010, J. Quant. Spec. Radiat. Transf., 111, 2151
Dubernet, M. L., Roueff, E., Stoecklin, T., Daniel, F., & Grosjean, A. 2011, in EAS Publ. Ser. 52, eds. M. Röllig, R. Simon, V. Ossenkopf, & J. Stutzki, 217
Dubernet, M. L., Nenadovic, L., & Doronin, M. 2012, in ASP Conf. Ser., TBD, ADASS XXI, eds. P. Ballester, & D. Egret (San Francisco: ASP), TBD
Dumouchel, F., Faure, A., & Lique, F. 2010, MNRAS, 406, 2488
Dumouchel, F., Kłos, J., & Lique, F. 2011, PCCP, 13, 8204
Endres, C., Giesen, T., Muller, H., et al. 2011, in IAU Symp., 280, 333
Faure, A., & Josselin, E. 2008, A&A, 492, 257
Faure, A., & Tennyson, J. 2001, MNRAS, 325, 443
Faure, A., & Tennyson, J. 2003, MNRAS, 340, 468
Faure, A., Gorfinkiel, J. D., & Tennyson, J. 2004a, MNRAS, 347, 323
Faure, A., Gorfinkiel, J. D., & Tennyson, J. 2004b, J. Phys. B: At. Mol. Opt. Phys., 37, 801
Faure, A., Valiron, P., Wernli, M., et al. 2005, J. Chem. Phys., 122, 221102
Faure, A., Kokoouline, V., Greene, C. H., & Tennyson, J. 2006, J. Phys. B: At. Mol. Opt. Phys., 39, 4261
Faure, A., Crimier, N., Ceccarelli, C., et al. 2007a, A&A, 472, 1029
Faure, A., Varambhia, H. N., Stoecklin, T., & Tennyson, J. 2007b, MNRAS, 382, 840

Faure, A., Wiesenfeld, L., Scribano, Y., & Ceccarelli, C. 2012, MNRAS, 420, 699
Flower, D. 2007, Molecular Collisions in the Interstellar Medium, 2nd edn. (Cambridge Astrophysics Series), 196
Flower, D. R. 1999a, J. Phys. B At. Mol. Opt. Phys., 32, 1755
Flower, D. R. 1999b, MNRAS, 305, 651
Flower, D. R. 2001a, J. Phys. B At. Mol. Opt. Phys., 34, 2731
Flower, D. R. 2001b, MNRAS, 328, 147
Flower, D. R., & Pineau des Forêts, G. 2012, MNRAS, 421, 2786
Flower, D. R., & Roueff, E. 1998a, J. Phys. B At. Mol. Opt. Phys., 31, L955
Flower, D. R., & Roueff, E. 1998b, J. Phys. B At. Mol. Opt. Phys., 31, 2935
Flower, D. R., & Roueff, E. 1999a, MNRAS, 309, 833
Flower, D. R., & Roueff, E. 1999b, J. Phys. B At. Mol. Opt. Phys., 32, 3399
Flower, D. R., Roueff, E., & Zeippen, C. J. 1998, J. Phys. B At. Mol. Opt. Phys., 31, 1105
Flower, D. R., Gourhis, G., & Launay, J.-M. 2000, Comp. Phys. Comm., 131, 187
Forrey, R. C., Balakrishnan, N., Dalgarno, A., & Lepp, S. 1997, ApJ, 489, 1000
Garrison, B. J., & Lester, W. A. 1975, J. Chem. Phys., 63, 1449
Gianturco, F. A., & Jain, A. 1986, Phys. Rep., 143, 347
Ginard, D., González-García, M., Fuente, A., et al. 2012, A&A, 543, A27
Green, S. 1975, ApJ, 201, 366
Green, S. 1989, ApJS, 70, 813
Green, S. 1991, ApJS, 76, 979
Green, S. 1994, ApJ, 434, 188
Green, S. 1995, ApJS, 100, 213
Green, S., & Chapman, S. 1978, ApJS, 37, 169
Green, S., & Thaddeus, P. 1974, ApJ, 191, 653
Green, S., Defrees, D. J., & McLean, A. D. 1987, ApJS, 65, 175
Green, S., Maluendes, S., & McLean, A. D. 1993, ApJS, 85, 181
Groenenboom, G. C., & Struniewicz, I. M. 2000, J. Chem. Phys., 113, 9562
Hammami, K., Lique, F., Jaïdane, N., et al. 2007, A&A, 462, 789
Hammami, K., Nkem, C., Owono Owono, L. C., Jaidane, N., & Ben Lakhdar, Z. 2008, J. Chem. Phys., 129, 204305
Hammami, K., Owono, L. O., Jaidane, N., & Lakhdar, Z. B. 2008a, J. Mol. Struct.: THEOCHEM, 853, 18
Hammami, K., Owono, L. O., Jaidane, N., & Lakhdar, Z. B. 2008b, J. Mol. Struct.: THEOCHEM, 860, 45
Hammami, K., Owono Owono, L. C., & Stäuber, P. 2009, A&A, 507, 1083
Heijmen, T., Moszynski, R., Wormer, P., & Van der Avoird, A. 1996, Mol. Phys., 89, 81
Heijmen, T., Korona, T., Moszynski, R., Wormer, P., & Van der Avoird, A. 1997a, J. Chem. Phys., 107, 902
Heijmen, T., Moszynski, R., Wormer, P., & Van der Avoird, A. 1997b, J. Chem. Phys., 107, 9921
Heijmen, T. G. A., Moszynski, R., Wormer, P. E. S., & van der Avoird, A. 1997c, J. Chem. Phys., 107, 9921
Heijmen, T., Moszynski, R., Wormer, P., et al. 1999a, J. Chem. Phys., 111, 2519
Heijmen, T., Wormer, P., Van der Avoird, A., Miller, R., & Moszynski, R. 1999b, J. Chem. Phys., 110, 5639
Higgins, K., & Klemperer, W. 1999, J. Chem. Phys., 110, 1383
Hodges, M. P., & Wheatley, R. J. 2001, J. Chem. Phys., 114, 8836
Hutson, J. M., & Green, S. 1994, MOLSCAT computer code, version 14 (UK: Collaborative Computational Project No. 6 of the Science and Engineering Research Council)
Itikawa, Y. 2004, J. Phys. B: At. Mol. Opt. Phys., 37, R1
Itikawa, Y., & Mason, N. 2005, Phys. Rep., 414, 1
Jankowski, P., & Szalewicz, K. 1998, J. Chem. Phys., 108, 3554
Jankowski, P., McKellar, A., & Szalewicz, K. 2012, science, 336, 1147
Jaquet, R., Staemmler, V., Smith, M. D., & Flower, D. R. 1992, J. Phys. B At. Mol. Opt. Phys., 25, 285
Jeziorski, B., Moszyński, R., & Szalewicz, K. 1994, Chem. Rev., 94, 1887
Kalemos, A., Mavridis, A., & Metropoulos, A. 1999, J. Chem. Phys., 111, 9536
Kalugina, Y., Lique, F., & Kłos, J. 2012, MNRAS, 2545
Keller, H.-M., Floethmann, H., Dobbyn, A. J., et al. 1996, J. Chem. Phys., 105, 4983
Kłos, J., & Lique, F. 2008, MNRAS, 390, 239
Kłos, J., & Lique, F. 2011, MNRAS, 418, 271
Kłos, J., Chalasinski, G., Berry, M. T., Bukowski, R., & Cybulski, S. M. 2000, J. Chem. Phys., 112, 2195
Kłos, J., Lique, F., & Alexander, M. H. 2007, Chem. Phys. Lett., 445, 12
Kłos, J., Lique, F., & Alexander, M. H. 2008, Chem. Phys. Lett., 455, 1
Kłos, J., Lique, F., & Alexander, M. H. 2009, Chem. Phys. Lett., 476, 135
Kokoouline, V., Faure, A., Tennyson, J., & Greene, C. H. 2010, MNRAS, 405, 1195
Kouri, D. J. 1979, in Atom-molecule collision theory: a guide for the experimentalist, ed. R. B. Bernstein (New York: Plenum Press), 259
Krupnov, A. F. 2010, Phys. Rev. A, 82, 6703

Launay, J. M., & Roueff, E. 1977, A&A, 56, 289

Lee, H., McCoy, A. B., Toczyłowski, R. R., & Cybulski, S. M. 2000, J. Chem. Phys., 113, 5736

Light, J. C. 1979, in Atom-molecule collision theory: a guide for the experimentalist, ed. R. B. Bernstein (New York: Plenum Press), 239

Lim, A. J., Rabadán, I., & Tennyson, J. 1999, MNRAS, 306, 473

Lique, F. 2010, J. Chem. Phys., 132, 4311

Lique, F., & Kłos, J. 2011, MNRAS, 413, L20

Lique, F., & Spielfiedel, A. 2007, A&A, 462, 1179

Lique, F., Spielfiedel, A., Dubernet, M.-L., & Feautrier, N. 2005, J. Chem. Phys., 123, 134316

Lique, F., Dubernet, M.-L., Spielfiedel, A., & Feautrier, N. 2006a, A&A, 450, 399

Lique, F., Spielfiedel, A., & Cernicharo, J. 2006b, A&A, 451, 1125

Lique, F., Spielfiedel, A., Dhont, G., & Feautrier, N. 2006c, A&A, 458, 331

Lique, F., Senent, M.-L., Spielfiedel, A., & Feautrier, N. 2007, J. Chem. Phys., 126, 164312

Lique, F., Kłos, J., & Hochlaf, M. 2010a, PCCP, 12, 15672

Lique, F., Spielfiedel, A., Feautrier, N., et al. 2010b, J. Chem. Phys., 132, 4303

Machin, L., & Roueff, E. 2005, J. Phys. B At. Mol. Opt. Phys., 38, 1519

Machin, L., & Roueff, E. 2006, A&A, 460, 953

Machin, L., & Roueff, E. 2007, A&A, 465, 647

Maluendes, S., McLean, A. D., & Green, S. 1992, J. Chem. Phys., 96, 8150

Maret, S., Faure, A., Scifoni, E., & Wiesenfeld, L. 2009, MNRAS, 399, 425

McBane, G. 2004, MOLSCAT computer code, parallel version (USA: G. McBane)

McGuire, P., & Kouri, D. J. 1974, J. Chem. Phys., 60, 2488

Miller, R., Heijmen, T., Wormer, P., Van der Avoird, A., & Moszynski, R. 1999, J. Chem. Phys., 110, 5651

Monteiro, T. 1984, MNRAS, 210, 1

Monteiro, T. S. 1985, MNRAS, 214, 419

Monteiro, T. S., & Stutzki, J. 1986, MNRAS, 221, 33P

Moreau, N., & Dubernet, M. L. 2006a, in SF2A-2006: Semaine de l'Astrophysique Francaise, eds. D. Barret, F. Casoli, G. Lagache, A. Lecavelier, & L. Pagani, 95

Moreau, N., & Dubernet, M. L. 2006b, in Astronomical Data Analysis Software and Systems XV, eds. C. Gabriel, C. Arviset, D. Ponz, & S. Enrique, ASP Conf. Ser., 351, 391

Moszynski, R., Korona, T., Wormer, P., & Van der Avoird, A. 1997, jpca, 101, 4690

Muchnick, P., & Russek, A. 1994, J. Chem. Phys., 100, 4336

Müller, H. S. P., Schlöder, F., Stutzki, J., & Winnewisser, G. 2005, J. Mol. Struct., 742, 215

Müller, H. S. P., Thorwirth, S., Roth, D. A., & Winnewisser, G. 2001, A&A, 370, L49

Neufeld, D. A., & Green, S. 1994, ApJ, 432, 158

Neufeld, D. A., González-Alfonso, E., Melnick, G., et al. 2011, ApJ, 727, L29

Nisini, B., Benedettini, M., Codella, C., et al. 2010, A&A, 518, L120

Nkem, C., Hammami, K., Manga, A., et al. 2009, J. Mol. Struct.: Theochem., 901, 220

Pack, R. T. 1974, J. Chem. Phys., 60, 633

Palma, A. 1987, ApJS, 64, 565

Palma, A., & Green, S. 1987, ApJ, 316, 830

Palma, A., Green, S., Defrees, D. J., & McLean, A. D. 1988, J. Chem. Phys., 89, 1401

Parlant, G., & Yarkony, D. R. 1999, J. Chem. Phys., 110, 363

Patel, N. A., Young, K. H., Gottlieb, C. A., et al. 2011, ApJS, 193, 17

Pattengill, M. D. 1979, in Atom-molecule collision theory: a guide for the experimentalist, ed. R. B. Bernstein (New York: Plenum Press), 265

Phillips, T. R., Maluendes, S., & Green, S. 1996, ApJS, 107, 467

Phillips, T. R., Maluendes, S., McLean, A. D., & Green, S. 1994, J. Chem. Phys., 101, 5824

Pickett, H. M., Poynter, R. L., Cohen, E. A., et al. 1998, J. Quant. Spectrosc., & Rad. Transfer, 60, 883

Pottage, J. T., Flower, D. R., & Davis, S. L. 2002, J. Phys. B: At. Mol. Opt. Phys., 35, 2541

Pottage, J. T., Flower, D. R., & Davis, S. L. 2004, MNRAS, 352, 39

Rabadan, I., Sarpal, B. K., & Tennyson, J. 1998, MNRAS, 299, 171

Rabitz, H. 1976, in Dynamics of Molecular Collisions, Part A, ed. W. H. Miller (New York: Plenum Press), 33

Rabli, D., & Flower, D. R. 2010a, MNRAS, 406, 95

Rabli, D., & Flower, D. R. 2010b, MNRAS, 403, 2033

Rabli, D., & Flower, D. R. 2011, MNRAS, 411, 2011

Reese, C., Stoecklin, T., Voronin, A., & Rayez, J. C. 2005, A&A, 430, 1139

Rixon, G., Dubernet, M. L., Piskunov, N., et al. 2011, in AIP Conf. Ser., 1344, eds. A. Bernotas, R. Karazija, & Z. Rudzikas, 107

Rothman, L. S., Gordon, I. E., Barbe, A., et al. 2009, JQSRT, 110, 533

Roueff, E., & Flower, D. R. 1999, MNRAS, 305, 353

Roueff, E., & Zeippen, C. J. 1999, A&A, 343, 1005

Royer, P., Decin, L., Wesson, R., et al. 2010, A&A, 518, L145

Sarpal, B. K., & Tennyson, J. 1993, MNRAS, 263, 909

Sarrasin, E., Abdallah, D. B., Wernli, M., et al. 2010, MNRAS, 404, 518

Schöier, F. L., van der Tak, F. F. S., van Dishoeck, E. F., & Black, J. H. 2005, A&A, 432, 369

Schröder, K., Staemmler, V., Smith, M. D., Flower, D. R., & Jaquet, R. 1991, J. Phys. B At. Mol. Opt. Phys., 24, 2487

Schwenke, D. W. 1988, J. Chem. Phys., 89, 2076

Secrest, D. 1975, J. Chem. Phys., 62, 710

Secrest, D. 1979, in Atom-molecule collision theory: a guide for the experimentalist, ed. R. B. Bernstein (New York: Plenum Press), 265

Shafir, D., Novotny, S., Buhr, H., et al. 2009, Phys. Rev. Lett., 102, 223202

Spielfiedel, A., Senent, M.-L., Dayou, F., et al. 2009, J. Chem. Phys., 131, 014305

Spielfiedel, A., Feautrier, N., Najar, F., et al. 2012, MNRAS, 421, 1891

Staemmler, V., & Flower, D. R. 1991, J. Phys. B At. Mol. Opt. Phys., 24, 2343

Stoecklin, T., Voronin, A., & Rayez, J. C. 2003, Chem. Phys., 294, 117

Tennyson, J. 2010, Phys. Rep., 491, 29

Tercero, B., Vincent, L., Cernicharo, J., Viti, S., & Marcelino, N. 2011, A&A, 528, A26

Toboła, R., Kłos, J., Lique, F., Chałasiński, G., & Alexander, M. H. 2007, A&A, 468, 1123

Toboła, R., Lique, F., Kłos, J., & Chałasiński, G. 2008, J. Phys. B At. Mol. Opt. Phys., 41, 155702

Toboła, R., Dumouchel, F., Kłos, J., & Lique, F. 2011, J. Chem. Phys., 134, 4305

Toczyłowski, R. R., Doloresco, F., & Cybulski, S. M. 2001, J. Chem. Phys., 114, 851

Troscompt, N., Faure, A., Wiesenfeld, L., Ceccarelli, C., & Valiron, P. 2009, A&A, 493, 687

Tsien, T. P., & Pack, R. T. 1970a, Chem. Phys. Lett., 6, 54

Tsien, T. P., & Pack, R. T. 1970b, Chem. Phys. Lett., 6, 400

Turner, B. E., Chan, K.-W., Green, S., & Lubowich, D. A. 1992, ApJ, 399, 114

Turpin, F., Stoecklin, T., & Voronin, A. 2010, A&A, 511, A28

Valiron, P., Wernli, M., Faure, A., et al. 2008, J. Chem. Phys., 129, 134306

van der Tak, F., Black, J., Schöier, F., Jansen, D., & van Dishoeck, E. 2007, A&A, 468, 627

Varambhia, H. N., Gupta, M., Faure, A., Baluja, K. L., & Tennyson, J. 2009, J. Phys. B At. Mol. Opt. Phys., 42, 095204

Vincent, L. F. M., Spielfiedel, A., & Lique, F. 2007, A&A, 472, 1037

Werner, H.-J., Knowles, P. J., Knizia, G., Manby, F. R., & Schütz, M. 2012, WIREs Comput Mol Sci, 2, 242

Wernli, M., Valiron, P., Faure, A., et al. 2006, A&A, 446, 367

Wernli, M., Wiesenfeld, L., Faure, A., & Valiron, P. 2007a, A&A, 464, 1147

Wernli, M., Wiesenfeld, L., Faure, A., & Valiron, P. 2007b, A&A, 475, 391

Wiesenfeld, L., & Faure, A. 2010, Phys. Rev. A, 82, 040702

Yang, B., Stancil, P. C., Balakrishnan, N., & Forrey, R. C. 2010, ApJ, 718, 1062

Yau, A. W., & Dalgarno, A. 1976, ApJ, 206, 652

Zernickel, A., Schilke, P., Schmiedeke, A., et al. 2012, A&A, 546, A87

Zhang, R., Faure, A., & Tennyson, J. 2009, Phys. Scr., 80, 5301