Transactions IAU, Volume XXIXA
Proc. XXIXA IAU General Assembly, August 2015
Thierry Montmerle, ed.

doi:10.1017/S1743921316000697

DIVISION B
COMMISSION 14

ATOMIC AND MOLECULAR DATA
DONNÉES ATOMIQUES ET MOLÉCULAIRES

WORKING GROUP

COLLISION PROCESSES
PROCESSUS COLLISIONNELS

CO-CHAIRS

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TRIENNIAL REPORT 2012-2015

1. Introduction

Since our last report (Peach & Dimitrijević 2012), a large number of new publications on the results of research in atomic and molecular collision processes and spectral line broadening have been published. Due to the limited space available, we have only included work of importance for astrophysics. Additional relevant papers, not included in this report, can be found in the databases at the web addresses provided in Section 6. Elastic and inelastic collisions between electrons, atoms, ions, and molecules are included, as well as charge transfer in collisions between heavy particles which can be very important.

Numerous conferences on collision processes and line broadening have been held since our last report. Some important international meetings that publish proceedings where additional data and their sources can be found are:

The 21^{th} *International Conference on Spectral Line Shapes* (ICSLS) (Devdariani 2012), the 22^{th} ICSLS (Parigger 2014), the 8^{th} *Serbian Conference on Spectral Line Shapes in Astrophysics* (SCSLSA) (Popović *et al.* 2011), the 9^{th} SCSLSA (Popović 2014), the XXVII *International Conference on Photonic, Electronic, and Atomic Collisions* (ICPEAC) (Williams *et al.* 2012), the XXVIII ICPEAC (Guoqing Xiao 2014), the 23^{rd} *International Conference on Atomic Physics* (ICAP) (Dulieu *et al.* 2013), the 8^{th} *International Conference on Atomic and Molecular Data and their Applications* (ICAMDATA) (Gillaspy *et al.* 2013), 1^{st} *Spectral Line Shapes in Plasmas Code Comparison Workshop* (SLSP) (see review in Stambulchik 2013) and the 2^{nd} (SLSP) (Stambulchik *et al.* 2014). Selected papers from the 9^{th} ICAMDATA are in press in Physica Scripta.

2. Electron collisions with atoms, ions, molecules and molecular ions

Collisions of electrons with atoms, molecules and atomic and molecular ions are the major excitation mechanism for a wide range of astrophysical environments. In addition, electron collisions play an important role in ionization and recombination, contribute to cooling and heating of the gas, and may contribute to molecular fragmentation and formation. In the following sections we summarize recent work on collisions for

astrophysically relevant species, including elastic scattering, excitation, ionization, dissociation, recombination and electron attachment and detachment.

2.1. *Electron-atom scattering*

Extensive large-scale studies of elastic, excitation and ionisation cross sections for N (Wang *et al.* 2014b), F (Gedeon *et al.* 2014) and Ne (Zatsarinny & Bartschat 2012) have been presented. Elastic scattering has been studied for fine-structure resolved states of Cl (Wang *et al.* 2013c) as well as for Ca (Hasan *et al.* 2014), Mn (Dolmatov *et al.* 2013), In, Tl, Ga and At (Felfli *et al.* 2012), and Eu and Yb (Kelemen *et al.* 2013). New work on excitation includes: H (Vrinceanu *et al.* 2014), He in an electric field (Smirnov 2013), C including ionisation (Wang *et al.* 2013d), Ar (Zatsarinny *et al.* 2014), Zn (Das *et al.* 2012), Cs (Bostock *et al.* 2014), Yb (Das *et al.* 2012), and Pb (Zatsarinny *et al.* 2013).

2.2. *Electron-ion scattering*

Several large-scale efforts to calculate excitation data for iso-electronic sequences have been undertaken. For He-like ions data is now available covering most ions from Mg^{10+} to Kr^{34+} (Aggarwal & Keenan 2012b, Aggarwal & Keenan 2012d, Aggarwal & Keenan 2012e, Aggarwal & Keenan 2012c, Aggarwal & Keenan 2013b, Aggarwal & Keenan 2013c).

For Li-like ions data has been calculated for ions from Mg^9+ to Ni^{25+} (Aggarwal & Keenan 2012a, Aggarwal & Keenan 2013a). For Be-like ions data has been presented for ions from B^+ to Zn^{26+} (Fernández-Menchero *et al.* 2014a), and also Cl^{13+}, K^{15+} and Ge^{28+} (Aggarwal & Keenan 2014d) and Ti^{18+} (Aggarwal & Keenan 2012f). For B-like ions data covering from C^+ to Kr^{31+} (Liang *et al.* 2012), and also Al^{9+} (Aggarwal & Keenan 2014a), have been calculated. For Mg-like ions data covering from Al^+ to Zn^{18+} have been presented (Fernández-Menchero *et al.* 2014b).

Other new work on specific ions includes: $^3He^+$ and other one-electron ions (Bartschat & Sadeghpour 2014), O^{2+} (Palay *et al.* 2012, Storey *et al.* 2014), O^{4+} and O^{5+} (Elabidi & Sahal-Bréchot 2013), Ne^{4+} (Dance *et al.* 2013), Mg^{2+} and Al^{3+} (Elabidi 2014), Mg^{5+} (Tayal 2012a), Mg^{7+} (Grieve *et al.* 2013), Si^+ (Aggarwal & Keenan 2014b), Si^{6+} (Sossah & Tayal 2014), Si^{7+} (Tayal 2012b, Li *et al.* 2013), S^{2+} (Hudson *et al.* 2012b, Grieve *et al.* 2014), S^{14+} and S^{15+} including recombination (Mahmood *et al.* 2012), Cl^{2+} (Sossah & Tayal 2012), Ca^{13+} (Dong *et al.* 2012), Sc^+ (Grieve *et al.* 2012), Fe^{2+} (Badnell & Balance 2014), Fe^{6+} (Tayal & Zatsarinny 2014), Fe^{7+} (Del Zanna & Badnell 2014), Fe^{13+} (Aggarwal & Keenan 2014c), Ni^{13+} (Wang *et al.* 2012), Ni^{17+} (Hudson *et al.* 2012a), Ge^+ (Smirnov 2014), Nb^{+11} and Mo^{+12} (Liang *et al.* 2014), Sn^{13+} including ionization (Liu *et al.* 2014b), W^{3+} including ionisation (Ballance *et al.* 2013), and Au^{51+} (Fan *et al.* 2014).

2.3. *Electron-molecule and electron-molecular ion scattering*

For molecules, new work includes: H_2^+ including proton-production and dissociative ionisation (Zammit *et al.* 2013), H_2 including excitation and dissociation (Lan & Leon 2012, Wang *et al.* 2013a, Ki & Jung 2013), excitation of HD^+ (Motapon *et al.* 2014), dissociative ionisation of D_2 (Lower *et al.* 2013), dissociative recombination of LiH_2^+ (Thomas *et al.* 2014), excitation of BeH^+ (Chakrabarti & Tennyson 2012, Niyonzima *et al.* 2013), elastic, inelastic and total cross sections for HCN (Sanz *et al.* 2012), elastic and inelastic scattering on H_2CN (Wang it et al. 2014a), dissociative recombination of N_2^+ (Little *et al.* 2014), excitation and dissociation of N_2 (Malone *et al.* 2012, Laporta *et al.* 2014, Xin & Ding 2014), excitation of H_2O (Rescigno & Orel 2013), dissociative ionisation of HDO^+ (Defrance *et al.* 2014), elastic and inelastic scattering on CO (Laporta *et al.* 2012, Ristić *et al.* 2012, Wang *et al.* 2013b), dissociative recombination of

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HCO^+ and HOC^+ (Larson *et al.* 2012), elastic and inelastic scattering on NO (Chiari *et al.* 2013), total scattering and excitation cross sections for N_2O (Vinodkumar & Barot 2012, Watanabe & Takahashi 2014), elastic, excitation and ionisation cross sections for NCO (Kaur & Baluga 2012), elastic, excitation and ionisation processes on O_2 (Singh & Baluja 2014), fragmentation of CO_2^{2+} (Wang *et al.* 2014c), excitation of NF_3 (Goswami *et al.* 2013), and elastic scattering on OCS and CS_2 (Murai *et al.* 2013).

Regarding more complex molecules, new references include: dissociative electron attachment on acetone (Prabhudesai *et al.* 2014), excitation of allene (Barot *et al.* 2013), elastic and inelastic scattering on formamide (Wang & Tian 2012), dissociation of methane (Ziółkowski *et al.* 2012), elastic and inelastic scattering on pyrazine (Palihawadana *et al.* 2012, Sanz *et al.* 2013), elastic and inelastic scattering on pyrimidine (Mašín *et al.* 2012), and inelastic scattering on uracil (Shafranyosh & Sukhoviya 2012).

3. Heavy particle collisions

Collisions between heavy particles are important in many astrophysical environments, particularly those involving H and He as they are astrophysically abundant. In the following sections we attempt to summarise recent work on collisions for astrophysically relevant species, including excitation, ionisation and charge transfer. We note that a review of reactive scattering and chemistry relevant to astrophysics is beyond the scope of the present report.

3.1. *Atom-atom and ion-atom collisions*

Excitation and charge transfer in collisions of neutral atoms with hydrogen atoms are important processes in stellar atmospheres, and studies include: H + H and Be + H (Miyano Hedberg *et al.* 2014), Mg + H (Belyaev *et al.* 2012, Barklem *et al.* 2012), Al + H (Belyaev 2013a, Belyaev 2013b), Si + H (Belyaev *et al.* 2014b), and Cs + H (Belyaev *et al.* 2014a). Excitation and charge transfer in H + H^+ collisions have been studied (Tseliakhovich *et al.* 2012) and proton-Rydberg atom (Vrinceanu *et al.* 2012), atom-Rydberg atom (Srećković *et al.* 2013) collisions studied generally. Charge transfer, excitation and ionisation in collisions between ions and neutral atoms play important roles in a number of astrophysical environments. New work on processes involving hydrogen atoms and protons include: excitation, ionisation and charge transfer in collisions between protons and He^+, Li^{2+}, Be^{3+}, B^{4+}, and C^{5+} (Winter 2013), proton collisions with He (Liu *et al.* 2012), excitation and charge transfer in Li^{q+} + H collisions (Liu *et al.* 2014c), charge transfer in Be^{3+} + H collisions (Liu & Wang 2013), charge transfer and ionisation of Be, Fe, Mo and W by H collisions (Tolstikhina *et al.* 2014), charge transfer in C^{5+} + H collisions (Nolte *et al.* 2012b), charge transfer and ionisation in C^{6+}, N^{7+} + H collisions (Jorge *et al.* 2014), charge transfer in O^{6+} + H collisions (Wu *et al.* 2012), charge transfer and ionisation in O^{8+} + H collisions (Pandey *et al.* 2012), charge transfer and ionisation in He-like ions (Li^+, Be^{2+}, B^{3+}, C^{4+}, N^{5+}, O^{6+}) + H collisions (Pandey *et al.* 2013), charge transfer and ionisation in N^{7+}, N^{6+}, C^{6+} + H collisions (Igenbergs *et al.* 2012), charge transfer in Si^{3+} + H collisions (Liu *et al.* 2014a), charge transfer in Kr^{36+}, W^{60+} + H collisions (Illescas *et al.* 2013) and charge transfer of W^+ and W^{2+} with H and H_2 (Tolstikhina *et al.* 2012).

New references regarding charge transfer involving He and He^+ include: He^+ + He (Kusakabe *et al.* 2012), Li + He (Belyaev *et al.* 2014), Si + He^+ (Satta *et al.* 2013), C^{4+} + He collisions (Yan *et al.* 2013), O^{8+} + He collisions (Wang & Wang 2012), Ne^{10+} + He, Ne (Liu *et al.* 2014d). An overview of charge transfer and ionisation for heavy many-electron ions colliding with neutral atoms has been given in (Tolstikhina & Shevelko

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2013) and W^+, W^{2+} + He (Tolstikhina *et al.* 2012). A classical model for ion collisions with He atoms, including charge transfer and ionisation processes, has been presented (Ding 2012). Other references include studies of charge transfer of Ar with highly charged ions (Otranto *et al.* 2014), Ar^{16+} + Ne (Xue *et al.* 2014).

The study of polarisation in spectral lines requires information on the destruction of polarisation by collisions, including with H. Some recent studies include those of Derouich (2012), Deb & Derouich (2014) and Manso Sainz *et al.* (2014).

3.2. *Atom-, ion-, and molecule-molecule Collisions*

A second edition of the book *Molecular Collisions in the Interstellar Medium* (Flower 2012) has been published and also Roueff & Lique (2013) have published a review entitled *Molecular Excitation in the Interstellar Medium: Recent Advances in Collisional, Radiative and Chemical Processes*.

For excitation, new references include: CO + H^+, H_2^+, H_3^+ (Werbowy & Pranszke 2014), CO + H (Yang *et al.* 2013b), HD + He (Nolte *et al.* 2012a), OH^+ + He (Gómez-Carrasco *et al.* 2014), HCl + He (Lanza & Lique 2012, Yang & Stancil 2014), H_2O + He (Yang *et al.* 2013a), DCO^+ + He (Buffa 2012), C_2H + He (Spielfiedel *et al.* 2012), H_2CO + He (Sharma *et al.* 2014), H_2 + H_2 (Bohr *et al.* 2014), C^+ + H_2 (Wiesenfeld & Goldsmith 2014), CN + H_2 (Kalugina *et al.* 2012), O_2 + H_2 (Lique *et al.* 2014), HCO^+ + H_2 (Yazidi *et al.* 2014), NH_2D + H_2 (Daniel *et al.* 2014).

For charge transfer and related processes, new work includes: H^+, H_2^+, H_3^+ + CO (Werbowy & Pranszke 2014), charge transfer involving multiply charged ions and CO (Cariatore & Oranto 2013) charge transfer of He^+ with simple molecules (Kusakabe *et al.* 2012), single and multiple electron charge transfer and ionisation in H^++H_2O (Murakami *et al.* 2012a), as well as multiple electron removal and fragmentation processes in He^++H_2O collisions (Murakami *et al.* 2012b).

4. Stark broadening

Stark broadening parameters are required for the analysis, synthesis and interpretation of stellar spectra, and for other astrophysical plasmas, such as H I and H II regions or neutron stars. Data on line widths and shifts for a large number of atomic transitions are particularly important for hot dense stars such as white dwarfs, where Stark broadening is usually the most important broadening mechanism.

4.1. *Developments in line broadening theory*

Stambulchik & Maron (2013) have developed an analytical method based on the quasi-contiguous approximation to the static line shapes for Stark broadening of H and H-like transitions including Rydberg ones. The unified formalism for the modeling of hydrogen Stark line shapes has been reexamined by Rosato *et al.* (2013) and extended to non-binary interactions between an emitter and the surrounding perturbers. Oks (2015) has reexamined conventional theory for Stark broadening, and his new calculations for the H_α line show that the effect of the ion dynamics may be slightly smaller than was accepted, while the effect of the acceleration of perturbing electrons by the ion field in the vicinity of the radiating atom may be larger.

Alexiou (2013) has proposed the implementation in lineshape codes of the Frequency Separation Technique based on the separation of the slow and fast frequency components.

Kinetic quantum equations for a density matrix with collision integrals describing nonlinear effects in line wing spectra, have been derived by Parkhomenko & Shalagin (2011).

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Rosato *et al.* (2012) have investigated the influence of correlated emitter-perturber collisions on hydrogen lines using kinetic theory. They concluded that such collisions strongly affect the width and shape of the line profile in the core region where the dynamical effects are included using the frequency-fluctuation-model approach. Demura & Stambulchik (2014) have studied the assumption that the density matrix is diagonal for the calculation of spectral lineshapes and the effect of microfield rotation on Stark profiles. The electron-impact broadening of ion lines has been calculated by Naam *et al.* (2014) using trajectories modified by non-Newtonian mechanics and the Maxwell-Jüttner velocity distribution.

The effect of the microfield direction on line shapes has been investigated by Calisti *et al.* (2014) and the ion-dynamic effect has been also analyzed by Ferri *et al.* (2014). A stochastic microfield formulation to treat the effect of particle motion in the Stark broadening of ion lines is extended by Iglesias (2013) to include an external uniform static magnetic field. Efficient algorithms for calculations of Stark-Zeeman line profiles for both static and dynamic ions are presented. Chenini *et al.* (2011) have investigated the influence of a non-uniform microfield on the asymmetry of Ly_α in a dense plasma and Difallah *et al.* (2012) have studied the effect on its profile of an oscillating electric field.

Baclawski & Musielok (2013) have presented a new approach for the evaluation of asymmetry parameters, and Galtier *et al.* (2013) have investigated quantum mechanical interference effects in Stark broadening of intrashell transitions for dense plasma conditions. Problems arising from the ideal Coulomb plasma approximation have been analysed by Rosato *et al.* (2014) and Sapar & Poolamäe (2012) have derived new analytical series expansions for the hydrogenic line shape functions.

Sahal-Bréchot *et al.* (2014a) have reviewed and analyzed the semiclassical perturbation theory (SCP) in order to introduce the main approximations, give the formulae used in the SCP code and to better understand the validity conditions. A review of different models used for the calculation of Stark broadening is presented by Gigosos (2014).

4.2. *Isolated lines*

Stark broadening of isolated lines is dominated by plasma-electron impacts. Broadening parameters, Stark widths and shifts, have been determined theoretically for:

2 B III (Duan *et al.* 2014), 8 Si IV (Elabidi *et al.* 2012) 6 Ar XV (Elabidi *et al.* 2014) lines and for 7 Sr II lines in an ultracold neutral plasma (Duan *et al.* 2013), using a quantum-mechanical approach in all cases.

For 9 resonant Cr II multiplets (Simić *et al.* 2013), 114 Pb IV lines (Hamdi *et al.* 2013), 32 Ar III lines (Hamdi *et al.* 2014), 148 C II multiplets (Larbi-Terzi *et al.* 2012), and 36 B IV (Dimitrijević *et al.* 2014), new Stark broadening parameters are calculated using a semiclassical perturbation approach. A semiclassical method is also used for the N I $(^1D)3s^2D$ - $(^1D)3p^2D^o$ doubly excited transition.

The Li I 460.28 nm spectral line and its forbidden component has been investigated using computer simulation (Cvejić *et al.* 2014).

A semi-empirical approach, that uses Hartree-Fock relativistic wave functions and includes core polarization effects, has been applied to 237 Mg III (Colón *et al.* 2013), 111 Mg III (from configurations $2p^54f$, $2p^55f$ and $2p^55g$ - Moreno-Díaz *et al.* 2014), 148 Ca III (Alonso-Medina & Colón 2013), 467 Ca IV (Alonso-Medina & Colón 2014), and 72 lines of Pb V (Alonso-Medina & Colón 2012). A modified semi-empirical approach is used for 15 Nb III (Simić *et al.* 2014) lines.

Broadening parameters have been obtained experimentally for the following numbers of lines:

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Li I 460.28 nm line with forbidden component (Cvejić *et al.* 2014), 6 He I (Gigosos *et al.* 2014), 3 Mg I and 1 Mg II (Cvejić *et al.* 2013), 1 N I (Bartecka 2014), 4 Al II (Ćirišan *et al.* 2014), 126 Ar II (Djurović *et al.* 2013), 13 Ar II (Gajo *et al.* 2013), 11 Ca II (Aguilera *et al.* 2014a), 26 Fe II (Aguilera *et al.* 2011), 36 Fe II and 27 Ni II (Aragón *et al.* 2014a, Aragón *et al.* 2014b), 2 Cu I (Burger *et al.* 2014b), 22 Cu I and 100 Cu II (Skočić *et al.* 2013), 1 Hg I, 19 Hg II, 6 Hg III, and 4 Hg IV (Gavrilov *et al.* 2012), 2 In I (Burger *et al.* 2014a), 4 In III (Skočić *et al.* 2012), 53 Ni II (Aragón *et al.* 2013), and 83 Cr II (Aguilera *et al.* 2014b) spectral lines.

Regularities and systematic trends of Stark broadening parameters within various spectral series have been investigated for spectral lines of helium (Dojčinović *et al.* 2012), lithium (Dojčinović *et al.* 2013b), beryllium (Dojčinović *et al.* 2011), calcium Tapalaga *et al.* 2012), potassium (Jevtić *et al.* 2012), and within homologous spectral series of alkaline earth metals (Dojčinović *et al.* 2013a). The systematic trends obtained and data on regular behaviour within spectral series, can be of interest for the spectroscopic diagnostic of astrophysical plasmas, since this enables the estimation and prediction of missing Stark broadening parameters.

4.3. *Transitions in hydrogenic and helium-like systems*

The Stark-broadened profile of Ly_α has been obtained using *ab initio* simulation calculations by generating the electric microfield with a renewal process (Hammami *et al.* 2012). Also Stark broadening of H_β has been investigated for cold plasmas with low electron densities (Palomares *et al.* 2012).

New relativistic quantum mechanical calculations of Stark widths and shifts of He II spectral lines have been published (Duan *et al.* 2012).

The Stark broadening of He I lines 501.6, 667.8, 728.1, 388.9, 587.6, and 706.5 nm has been studied theoretically and experimentally (Gigosos *et al.* 2014). The theory uses computer simulations of the dynamics for noninteracting particles. Also broadening of He I 492.2 nm line has been investigated theoretically by computer simulation (Lara *et al.* 2012), and with its forbidden components experimentally (Ivković *et al.* 2013). New Stark broadening parameters have been calculated for the allowed 447.1 nm line and its forbidden component at 447.0 nm (Faye *et al.* 2011), as well as for the 388.9 nm line (Omar *et al.* 2014).

New calculations of complete Stark broadened profiles for 15 radio recombination lines of hydrogen with the principal quantum number of the upper level n between 102 and 274, have been performed recently (Peach 2014). Electron and proton impact has been included and it has again been confirmed that for the radio recombination lines electron-impact broadening is the dominant broadening mechanism.

5. Broadening by neutral atoms and molecules

The analysis of experimental molecular spectra in order to extract line shape parameters is often very difficult. Line shapes can be affected by collisional narrowing and the dependence of collisional broadening and shifting on molecular speed. When these effects are sufficiently important, fitting Voigt profiles to experimental spectra produces systematic errors in the parameters retrieved. Several theoretical papers have been published that address these problems of modelling and computation, see Kochanov (2011), Stace *et al.* (2012), Westberg *et al.* (2012), Kochanov (2013), Berk (2013), Protasevich (2013), Wcisło & Ciuryło (2013), Tran *et al.* (2013) and Wang *et al.* (2014).

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The applicability or otherwise of power-law relations to describe the temperature variations of the pressure broadening and shifts of atomic and molecular lines have been studied by Cybulski *et al.* (2013).

In the following sections the experimental (E) and theoretical (T) results selected have been confined to the basic atomic and molecular data required for a description of the pressure broadening and shift of lines and molecular bands.

5.1. *Broadening and shift of atomic lines*

Some new research has been published in the period 2012-2015 and the transitions studied together with the perturbing atoms or molecules are listed below.

He: self-broadening of 1s–2p and 2p–3s transitions (T) (Allard *et al.* 2013).
Li: broadening of lines by He (T) (Allard *et al.* 2014).
Li: broadening of lines by H_2 (T) (Allard 2014).
Na: broadening of lines by H_2 (T) (Allard *et al.* 2012).
K, Rb, Cs: broadening, shift and asymmetry of D_1 and D_2 lines by He, Ne, Ar (T) (Blank & Weeks 2014).
K, Rb: D_1 and D_2 lines broadened and shifted by ^{3}He, N_2 (E) (Kluttz *et al.* 2013).
K: D2 line broadened and shifted by He, Ne, Ar, Kr, Xe, N_2, CH_4, C_2H_6, C_3H_8, n-C_4H_{10} (E) (Pitz *et al.* 2014).
Rb: D1 line broadened and shifted by He, CH_4, C_2H_6, C_3H_8, n-C_4H_{10} (E) (Pitz *et al.* 2014).
Ca^+: broadening of lines by He (T) (Allard & Alekseev 2014).
Cd: blue and red wings of the 326.1nm line perturbed by He, Ne, Ar, Kr, Xe (E) (Roston & Helmi 2014).
Ag: D1 line broadened by He, Ar and N_2 (E) (Karaulanov *et al.* 2012).
Dispersion coefficients C_6, C_8 and C_{10} for interactions between H, Li, Na and K atoms (T) (Kar *et al.* 2013).
Broadening of radiative transitions in charge exchange collisions of one-electron atomic ions and bare nuclei, also H^- + H (T) (Devdariani 2014).

5.2. *Broadening and shift of molecular lines*

Much new data has been published since the last report was prepared. The molecules are listed below with their perturbing atomic or molecular species.

H_2-H_2: electric quadrupole transitions and collision-induced absorption (E) (Kassi & Campargue 2014).
H_2-H_2: collision-induced absorption (E) (Abu-Karma 2015).
H_2O: lines broadened and shifted by H_2 (E+T) (Drouin & Wiesenfekl 2012).
H_2O: broadened by He isotopes (E) (Campbell & Havey 2013).
H_2O: lines broadened by air (E) (Birk & Wagner 2012).
H_2O: intermolecular potentials; vibration bands broadened by He (T) (Petrova *et al.* 2013).
H_2O: self-broadened vibration-rotation line (E+T) (De Visia *et al.* 2011).
H_2O: self-broadened lines and broadened by air (E) (Ngo *et al.* 2012).
H_2O: self-broadened lines, pressure-induced shifts (T) (Ma *et al.* 2012).
H_2O: self-broadened water vapour continuum (T) (Klimeshima & Rodimova 2013).
H_2O: self-broadened water vapour continuum (E) (Ptashnik *et al.* 2013).
H_2O: water vapour continuum broadened by air (E) (Slocum *et al.* 2013).
H_2O: self-broadening coefficients for lines of $H_2^{16}O$, $H_2^{17}O$, $H_2^{18}O$, $HD^{16}O$ (E) (Regalia *et al.* 2014).

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H_2O: rotational band broadened by N_2 (T) (Lamouroux *et al.* 2012a).
H_2O, CO: lines broadened by H_2 (T) (Faure *et al.* 2013).
H_2CO: anomalous absorption in molecular lines (E) (Sharma *et al.* 2012).
HO_2: lines broadened by N_2, O_2 (E) (Mizoguchi *et al.* 2012).
HO_2: ν_3 band broadened by air (E) (Minamida & Tonokura 2014).
HDO: self-broadened lines (E) (Daumont *et al.* 2012).
$(H_2O)_2$: lines perturbed by H_2O (T) (Odintsova *et al.* 2014).
HCl, HBr: lines broadened and shifted by N_2 (E) (Asfin *et al.* 2012).
CH_4: self-broadened lines (E) (Bowl *et al.* 2012), (Čermák *et al.* 2012).
CH_4: self-broadened lines and broadening by N_2 (E) (Sanzharov *et al.* 2012).
CH_4: lines broadened and shifted by CH_4 and air (E) (Smith *et al.* 2014).
CH_4: collision-induced absorption (T) (El-Kader & Maroulis 2012).
CH_4: lines broadened by CO_2 (E) (Fissiaux *et al.* 2014b).
CH_4: lines broadened by H_2, N_2, O_2 (T) (Gabard 2013).
CH_4: lines broadened and shifted by N_2 (E) (Kapitanov *et al.* 2012), (Vispoel *et al.* 2014).
CH_4: line mixing and lines broadened by air (E) (Ghysels *et al.* 2014).
CH_4: lines broadened by N_2, Ne (E) (Kapitanov *et al.* 2013).
CH_3D: lines broadened and shifted by N_2, O_2, CO_2 (E) (Tang *et al.* 2013).
CH_3F: self-broadened lines (E) (Okabayashi *et al.* 2015).
CH_3Br: self-broadened lines and broadened by N_2 (E) (Bousseta *et al.* 2015).
CH_3Cl: self-broadened lines and broadened by N_2 (E+T) (Bray *et al.* 2012), (Bray *et al.* 2013a), (Bray *et al.* 2013b).
CH_3Cl: lines broadened by O_2 (E+T) (Buldyreva *et al.* 2013).
CH_3Cl: self-broadened lines (E+T) (Ramchani *et al.* 2013), (Ramchani *et al.* 2014).
CH_3Cl: lines broadened by CO_2 (E) (Dudaryonok *et al.* 2014).
C_2H_2: lines self-broadened and shifted (T) (Galalou & Aroui 2013).
C_2H_2: lines broadened by N_2 (E+T) (Hashemi *et al.* 2014).
C_2H_2: self-broadened lines and broadening by N_2, He, Ar (E) (Sajid *et al.* 2014).
C_2H_4: self-broadened lines (E) (Auwera *et al.* 2014).
CH_3OH: lines broadened by air (E) (Harrison *et al.* 2012).
CH_2CCH_2: self-broadened lines and broadened by N_2 (E) (Fissiaux *et al.* 2013), (Fissiaux *et al.* 2014a).
CO, CO_2: lines broadened by H_2 (E) (Padmanabham *et al.* 2014).
CO: self-broadened lines and broadened by air (E) (Devi *et al.* 2012a), (Devi *et al.* 2012b).
CO_2: self-broadened lines (E) (Delière *et al.* 2012).
CO_2: self-broadened lines (T) (Hartmann *et al.* 2013a).
CO_2: absorption coefficients at high temperature and Pressure (E) (Stefani *et al.* 2013).
CO_2: lines broadened and shifted by N_2 (T) (Gamache *et al.* 2012).
CO_2: lines broadened and shifted by O_2, air (T) (Lamouroux *et al.* 2012b).
CO_2: lines broadened and shifted by N_2, O_2, CO_2, air (T) (Gamache & Lamouroux 2013), (Gamache *et al.* 2014).
CO_2, C_2H_2, CO, HCl, HF: lines broadened by Ar (T) (Ivanov & Buzykin 2013).
Cs_2: lines broadened by He, Ne, Kr (Tshikala *et al.* 2012), (Tshikala *et al.* 2014).
N_2: self-broadened lines (T) (Thibault *et al.* 2012).
O_2: self-broadened lines (T) (Hartmann *et al.* 2013b).
O_2: lines broadened by air (E+T) (Lamouroux *et al.* 2014).
O_2: lines broadened by H_2O (E) (Drouin *et al.* 2014).
OCO: self-broadened band lines (E) (Ngo *et al.* 2014).
OCS: bands broadened and shifted by O_2 (E) (Galalou *et al.* 2013).
SO_2: lines broadened by H_2, N_2, O_2, He (E) (Cazzoli *et al.* 2012).

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NH_3: self-broadened lines (T) (Cherkasov 2014).
NH_3: self-broadened isolated rovibrational line (E+T) (Triki *et al.* 2012).
NH_3: lines broadened by N_2, O_2, CO_2, H_2O (E) (Owen *et al.* 2013).
PH_3: lines self-broadened and shifted (E) (Devi *et al.* 2014).
PH_3: perturbed by H_2, line-mixing coefficients (E) (Salem *et al.* 2014).

6. Databases

The previous list of useful databases (Peach & Dimitrijević 2012) is updated, changes of web adresses are checked and the corresponding new references added. The selected databases are:

Vienna Atomic Line Database (VALD) is a collection of atomic and molecular transition parameters of astronomical interest for the analysis of radiation from astrophysical objects, containing central wavelengths, energy levels, statistical weights, transition probabilities and line broadening parameters for all chemical elements of astronomical importance. The newest version VALD3 can be found at http://vald.astro.uu.se/ (Kupka *et al.* 1999, Kupka *et al.* 2011).

CHIANTI database (Dere *et al.* 2009, Landi *et al.* 2012, Landi *et al.* 2013) contains a critically evaluated set of up-to-date atomic data for the analysis of optically thin collisionally ionized astrophysical plasmas. It lists experimental and calculated wavelengths, radiative data and rates for electron and proton collisions, see http://www.chiantidatabase.org/.

CDMS – Cologne Database for Molecular Spectroscopy, see website http://www.ph1.uni-koeln.de/vorhersagen/, provides recommendations for spectroscopic transition frequencies and intensities for atoms and molecules of astronomical interest in the frequency range 0-10 THz, i.e. 0-340 cm^{-1} (Müller *et al.* 2005).

BASECOL database (Dubernet *et al.* 2006, Dubernet *et al.* 2011b, Dubernet *et al.* (2013)), see website http://basecol.obspm.fr, is devoted to collisional rovibrational excitation of molecules by atoms, ions, molecules or electrons. It contains excitation rate coefficients for rovibrational excitation of molecules by electrons, He and H_2 and it is mainly used for the study of interstellar, circumstellar and cometary atmospheres.

TIPTOPbase (http://cdsweb.u-strasbg.fr/topbase/home.html) contains:
(i) TOPbase (Cunto & Mendoza 1992, Cunto *et al.* 1993), that lists atomic data computed in the Opacity and IRON Projects; namely *LS*-coupling energy levels, *gf*-values and photoionization cross sections for light elements ($Z \leqslant 26$) of astrophysical interest and large datasets of *f*-values for ions of Fe with configurations $3s^x 3p^y 3d^z$. (ii) TIPbase (Nahar 2003) contains fine-structure atomic data computed for ions of astrophysical interest in the IRON Project: radiative transition probabilities, electron impact excitation cross sections and rates for fine-structure transitions.

HITRAN – (HIgh-resolution TRANsmission molecular absorption database) is at http://www.cfa.harvard.edu/hitran/ (Rothman *et al.* 2009, Rothman *et al.* 2013, Hill *et al.* 2013). It lists individual line parameters for molecules in the gas phase (microwave through to the UV), photoabsorption cross-sections for many molecules, and refractive indices of several atmospheric aerosols. A high temperature extension to HITRAN is the High-temperature molecular spectroscopic database - HITEMP (To access the HITEMP data: ftp to cfa-ftp.harvard.edu; user = anonymous; password = e-mail address; cd/pub/HITEMP-2010). It contains data for water, CO_2, CO, NO and OH (Rothman *et al.* 2010).

GEISA – (Gestion et Etude des Informations Spectroscopiques Atmosphériques) is a computer-accessible spectroscopic database, designed to facilitate accurate forward

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radiative transfer calculations using a line-by-line and layer-by-layer approach. It can be found at http://ether.ipsl.jussieu.fr/etherTypo/?id=950 (Jacquinet-Husson *et al.* 2008, Jacquinet-Husson *et al.* 2011). The current 2011 edition of GEISA is a system comprising three independent sub-databases devoted respectively to: (i) Line transition parameters, (ii) Absorption cross-sections and (iii) Microphysical and optical properties of atmospheric aerosols.

NIST – The National Institute of Standards and Technology hosts a number of useful databases for Atomic and Molecular Physics. A list can be found at http://www.nist.gov/srd/atomic.cfm. Among them are: An atomic spectra database (http://www.nist.gov/pml/data/asd.cfm) and three bibliographic databases providing references on atomic energy levels and spectra (http://physics.nist.gov/cgi-bin/ASBib1/ELevBib.cgi), transition probabilities (http://physics.nist.gov/cgi-bin/ASBib1/TransProbBib.cgi) and spectral line shapes and line broadening (http://physics.nist.gov/cgi-bin/ASBib1/LineBroadBib.cgi).

STARK-B database (http://stark-b.obspm.fr) contains theoretical widths and shifts of isolated lines of atoms and ions due to collisions with charged perturbers, obtained using the impact approximation (Sahal-Bréchot 2010, Sahal-Bréchot *et al.* 2012, Sahal-Bréchot *et al.* 2014b).

BEAMBD – Belgrade electron/atom(molecule) database (Marinković *et al.* 2015 at http://servo.aob.rs/emol/). Contains electron interaction cross-sections for elastic scattering, electron excitation, ionization and total scattering.

The Virtual Atomic and Molecular Data Centre (VAMDC - http://www.vamdc.org/ - Dubernet *et al.* 2011a, Rixon *et al.* 2011) provides the international research community with access to a broad range of atomic and molecular (A&M) data compiled within a set of A&M databases (including all the above mentioned except NIST) accessible through the provision of a single portal.

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https://doi.org/10.1017/S1743921316000697 Published online by Cambridge University Press

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