

DIVISION XII / COMMISSION 14 / WORKING GROUP COLLISION PROCESSES

CO-CHAIRS

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TRIENNIAL REPORT 2009–2012

1. Introduction

Research in atomic and molecular collision processes and spectral line broadening has been very active since our last report, Peach, Dimitrijević & Stancil 2009. Given the large volume of the published literature and the limited space available, we have attempted to identify work most relevant to astrophysics. Since our report can not be comprehensive, additional publications can be found in the databases at the web addresses listed in the final section. Elastic and inelastic collisions among electrons, atoms, ions, and molecules are included and charge transfer can be very important in collisions between heavy particles.

Numerous meetings on collision processes and line broadening have been held throughout the report period. Important international meetings that provide additional sources of data through their proceedings are: the 19th *International Conference on Spectral Line Shapes (ICSLS)* (Gigosos & González 2008), the 7th *Serbian Conference on Spectral Line Shapes in Astrophysics (SCSLSA)* (Popović & Dimitrijević 2009), the XXVI *International Conference on Photonic, Electronic, and Atomic Collisions (ICPEAC)* (Orel *et al.* 2009), the 20th *ICSLS* (Lewis & Predoi-Cross 2010), the 22nd *International Conference on Atomic Physics (ICAP)* (Bachor, Drummond & Hannaford 2011), and the 7th *International Conference on Atomic and Molecular Data and their Applications* (Bernotas, Karazija & Rudzikas 2011). The 8th *SCSLSA* and the XXVIIth *ICPEAC* took place in June and July 2011 and their proceedings will be published in *Baltic Astronomy* and *Journal of Physics: Conference Series*, respectively.

2. Electron collisions with atoms and molecules

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.

A review has been published of the atomic data necessary for the non-LTE analysis of stellar spectra (Mashonkina 2009). Other references are listed below for scattering by the atoms and molecules specified.

2.1. *Electron scattering by neutral atoms*

Elastic scattering: H (screened Coulomb interactions) (Zhang *et al.* 2010), Mg (Zatsarinny *et al.* 2009), Ar (Gargioni & Grosswendt 2008), I (Zatsarinny *et al.* 2011), Mn, Cu, Zn,

Ni, Ag, Cd (Felfli *et al.* 2011), Rb, Cs, Fr (Gangwar *et al.* 2010).

Excitation: H (screened Coulomb interactions) (Zhang *et al.* 2010, Zhang *et al.* 2011), He($2^1,3S$) (Wang *et al.* 2009, Wang *et al.* 2010), He, Ne (Kretinin *et al.* 2008), Mg (Zatsarinny *et al.* 2009), Ar (Gargioni & Grosswendt 2008).

Ionization: He (Bray *et al.* 2010, Ren *et al.* 2011), He(2^1S) (Wang *et al.* 2010), Ar (Gargioni & Grosswendt 2008).

Total cross section: Na (Jiao *et al.* 2010).

2.2. Electron scattering by atomic ions

Elastic scattering: Mg⁺, Ca⁺ (Mitroy & Zhang 2008).

Excitation: Hydrogen isoelectronic sequence Cr²³⁺–Ni²⁷⁺ (Malespin *et al.* 2011), Lithium isoelectronic sequence Be⁺–Kr³³⁺ (Liang & Badnell 2011), Ne³⁺, Ne⁶⁺ (Ludlow *et al.* 2011), Neon isoelectronic sequence Na⁺–Kr²⁶⁺ (Liang & Badnell 2010), Sodium isoelectronic sequence Mg⁺–Kr²⁵⁺ (Liang *et al.* 2009b), Mg⁴⁺ (Hudson *et al.* 2009), Mg⁸⁺ (Del Zanna *et al.* 2008), Si⁹⁺ (Liang *et al.* 2009a), S⁸⁺–S¹¹⁺ (Liang *et al.* 2011), K⁺ (Tayal & Zatsarinny 2010), Fe¹⁰⁺ (Del Zanna *et al.* 2010), Fe¹²⁺ (Storey & Zeppen 2010), Fe¹⁸⁺ (Butler & Badnell 2008), Ni¹⁰⁺ (Aggarwal & Keenan 2008a), Ni¹⁸⁺ (Aggarwal & Keenan 2008c).

Recombination: H⁺ (Chluba *et al.* 2010), N⁺ (Fang *et al.* 2011), Aluminium isoelectronic sequence Si⁺–Zn¹⁷⁺ (Abdel-Naby *et al.* 2011), Argon isoelectronic sequence K⁺–Zn¹²⁺ (Nikolić *et al.* 2010), Fe⁷⁺, Fe⁸⁺ (Schmidt *et al.* 2008), Selenium ions Se^{q+}, $q = 1 - 6$ (Sterling & Witthoef 2011).

Energy levels, radiative and excitation rates: O³⁺ (Aggarwal & Keenan 2008b, Keenan *et al.* 2009), O⁶⁺ (Aggarwal & Keenan 2008d), Si⁺ (Bautista *et al.* 2009), Ar¹⁷⁺ (Aggarwal *et al.* 2008), Selenium ions Se^{q+}, $q = 1 - 6$ (Sterling & Witthoef 2011).

X-ray line emission: Na⁹⁺ (Phillips *et al.* 2010).

Radiative and Auger decay: Aluminium ions Al^{q+}, $q = 0 - 11$ (Palmeri *et al.* 2011).

2.3. Electron scattering by molecules

Elastic scattering: H₂O (Liu & Zhou 2010), (H₂O)₂ (Bouchiha *et al.* 2008), Li₂ (Tarana & Tennyson 2008), CO (Allan 2010), NH (Rajvanshi & Baluja 2010), NO₂ (Munjaj *et al.* 2009), S₂ (Rajvanshi & Baluja 2011), SO₂ (Machado *et al.* 2011), SOS (Kaur *et al.* 2010), S₃ (Kaur *et al.* 2011).

Electron exchange: O₂, NO, NO₂ (Holtkötter & Hanne 2009).

Excitation: H₂ (Kretinin *et al.* 2008), Li₂ (Tarana & Tennyson 2008), CO (Allan 2010), N₂ (Kato *et al.* 2010, Johnson *et al.* 2010, Mavadat *et al.* 2011), NH (Rajvanshi & Baluja 2010), NO₂ (Munjaj *et al.* 2009), S₂ (Rajvanshi & Baluja 2011), SOS (Kaur *et al.* 2010), S₃ (Kaur *et al.* 2011), C₂H₄ (da Costa *et al.* 2008).

Ionization: N₂ (Gochitashvili *et al.* 2010), NH (Rajvanshi & Baluja 2010), SiCl, SiCl₂, SiCl₃, SiCl₄ (Kothari *et al.* 2011), SO, SO₂ (Vinodkumar *et al.* 2008), SOS (Kaur *et al.* 2010), S₂ (Rajvanshi & Baluja 2011), S₃ (Kaur *et al.* 2011).

Total cross sections: SO, SO₂, SO₂Cl₂, SO₂ClF, SO₂F₂ (Joshipura & Gangopadhyay 2008), SO₂ (Machado *et al.* 2011), C₂H₄O (Szmytkowski *et al.* 2008), CH₃OH, CH₃NH₂ (Vinodkumar *et al.* 2008).

Dissociative processes: H₂ (Celiberto *et al.* 2009, Bellm *et al.* 2010, Celiberto *et al.* 2011), HCl (Fedor *et al.* 2010), HCl, DCl, HBr, DBr (Fedor *et al.* 2008), C₂H₂ (Chourou & Orel 2008).

Attachment: C_2H , C_2N (Harrison & Tennyson 2011).

2.4. Electron scattering by molecular ions

Detachment: C_2^- (Halmová *et al.* 2008).

Excitation: C_2^- (Halmová *et al.* 2008), CO^+ (Stäuber & Bruderer 2009).

Rotational cooling: HD^+ (Shafir *et al.* 2009).

Dissociative and recombination processes: HD^+ (Fifrig & Stroe 2008, Takagi *et al.* 2009, Stroe & Fifrig 2011), H_3^+ (Glosík *et al.* 2009), HF^+ (Roos *et al.* 2008, Roos *et al.* 2009), CH_3^+ , CD_3^+ (Bahati *et al.* 2009), $CD_3OCD_2^+$, $(CD_3)_2OD^+$ (Hamberg *et al.* 2010a), CD_3CDOD^+ , $CH_3CH_2OH_2^+$ (Hamberg *et al.* 2010b).

3. Collisions between heavy particles

A review entitled ‘Energetic ion, atom and molecule reactions and excitation in H_2 discharges’ has recently been published (Phelps 2009). Other references are listed below for the atomic and molecular processes specified.

3.1. Collisions between neutral atoms and atomic ions

Inelastic scattering: $H + H$ (Barklem *et al.* 2011), $Na + H$ (Barklem *et al.* 2010).

Excitation: $H + H^+$ (Winter 2009).

Charge transfer processes: $H, D, T + He^{2+}$ (Stolterfoht *et al.* 2010), $H^- + H^+$, mutual neutralization (Stenrup *et al.* 2009), $H + H^+$ (Winter 2009), $H + Li^{2+}$ (Mančev 2009), $H + B^{5+}, C^{4+}$ (Barragán *et al.* 2010), $H + C^{3+}, O^{3+}, Si^{3+}$ (Guevara *et al.* 2011), $H^+ + Li^+, Be^{2+}, B^{3+}, C^{4+}$ (Samanta & Purkait 2011), $He + H^+$ (Guzmán *et al.* 2009, Harris *et al.* 2010, Fischer *et al.* 2010), $He + H^+, He^{2+}$ (Zapukhlyak & Kirchner 2009), $He + H^+, He^+, He^{2+}$ (Schöffler *et al.* 2009), $He + {}^3He^{2+}$ (Alessi *et al.* 2011), $He + He^{2+}, Li^+, Li^{2+}, Li^{3+}, C^{6+}, O^{8+}$ (Samanta *et al.* 2011), $He + C^{3+}$ (Wu *et al.* 2009b), $He + N^{3+}$ (Liu *et al.* 2011b), $He + O^{3+}$ (Kamber *et al.* 2008, Wu *et al.* 2009a), $He, Ne, Ar, Kr, Xe + C^{3+}$ (Santos *et al.* 2010), $He^+ + He^+$ (Mančev 2009),

$Li + H, H^+$ (Cabrera-Trujillo *et al.* 2008), $Li + H^+$ (Liu *et al.* 2011a), $Ne + C^{2+}, C^{3+}, O^{2+}, O^{3+}$ (Ding *et al.* 2008), $Na + H$ ion-pair production (Barklem *et al.* 2010), $Mg + H^+, He^{2+}$ (Kumari *et al.* 2011), $Mg + Cs^+$ (Sabido *et al.* 2008), $Ar + H^+$ (Cabrera-Trujillo *et al.* 2009), $Ar + O^{3+}$ (Kamber *et al.* 2008).

Ionization: $H + H^+$ (Winter 2009), $He + H^+$ (Guzmán *et al.* 2009), $He + He^{2+}$ (Ogurtsov *et al.* 2011), $He, Ne, Ar, Kr, Xe + H^+$ (Miraglia & Gravielle 2008), $He, Ne, Ar, Kr, Xe + C^{3+}$ (Santos *et al.* 2010), $Li^+, Na^+, K^+, Rb^+ + H^+$ (Miraglia & Gravielle 2008).

Detachment: $C^-, O^-, F^-, Na^-, Si^-, S^-, Cl^-, Ge^- + He, Ne, Ar$ (Jalbert *et al.* 2008), $F^-, Cl^-, Br^-, I^- + H^+$ (Miraglia & Gravielle 2008).

Energy loss and stopping cross sections: $Li + H, H^+$ (Cabrera-Trujillo *et al.* 2008), $H, D, T + He^{2+}$ (Cabrera-Trujillo *et al.* 2011).

3.2. Collisions between atoms and molecules

Dissociative processes: $H_2O + H^+$ (Monce *et al.* 2009), $H_2O + He^+$ (Garcia *et al.* 2008).

Radiative association: $H_2 + H^-$ (Ayouz *et al.* 2011).

Excitation and/or fragmentation: $CN^- + H_2$ (Agúndez *et al.* 2010), $CO^+ + H$ (Andersson *et al.* 2008), $CO_2^+ + He$ (González-Magaña *et al.* 2008), $CO^+ + H, H_2$ (Stäuber & Bruderer 2009).

Charge transfer processes: D_2 , O_2 , H_2O , $CO_2 + O^{3+}$ (Kamber *et al.* 2008), $H_2 + He^{2+}$ (Khoma *et al.* 2009), $CH_3 + H^+$ (Nagao *et al.* 2008), $CO_2 + He^+$ (Lin & Mayer 2010), $HCl + C^{2+}$ (Rozsályi *et al.* 2011).

Ionization and/or capture: $H_2O + H^+$, He^{2+} , C^{6+} (Illescas *et al.* 2011), $C_2H_4 + H^+$ (Getahun *et al.* 2010), $N_2 + H^+$ (Gochitashvili *et al.* 2010).

4. Stark broadening

Knowledge of Stark broadening parameters (line widths and shifts) for a large number of atomic transitions is very important for the analysis, interpretation and modelling of stellar spectra, circumstellar conditions and H II regions. For hot dense stars such as white dwarfs this is often the most important broadening mechanism.

4.1. Developments in line broadening theory

Rosato *et al.* (2009) have reexamined the Stark broadening of hydrogen lines in the presence of a magnetic field and developed an impact theory for ions, valid for low electron densities ($N_e \leq 10^{14} \text{ cm}^{-3}$), which takes into account the Zeeman splitting of the atomic energy levels. Rosato *et al.* (2010) have also studied numerically the role of time ordering in such plasmas, by using a simulation code that accounts for the evolution of the microscopic electric field generated by the charged particles moving close to the atom. Calisti *et al.* (2010) have developed a very fast method to account for the dynamical effects of charged particles on the spectral line shape emitted by plasmas, based on a formulation of the frequency fluctuation model.

Ab initio calculations of Stark broadening parameters, i.e. calculations where the required atomic energy levels and oscillator strengths are determined during the calculation and are not taken from other sources, have been considered and reviewed by Ben Nessib (2009). A book has recently been published (Gordon & Sorochenko 2009) that gives a detailed account of the surprising discovery in the 1960's of the radio recombination lines and their subsequent analysis. Even now some features have still not been satisfactorily explained.

4.2. Isolated lines

For isolated lines Stark broadening is dominated by collisions with plasma electrons. Broadening parameters have been determined theoretically for:

One line from the 3s-3p transition array for each of the spectra Si XI, Ti XI, Cr XIII, Cr XIV, Fe XV, Fe XVI, Ni XVIII and Fe XXIII and two lines from the array for K VIII, Ca IX, Sc X and Ti XI (Elabidi & Sahal-Bréchet 2011); two lines for 3s-3p transitions for ions C IV, N V, O VI, F VII, Na IX, Mg X, Al XI, Si XII and P XIII and one line for Ne VIII (Elabidi *et al.* 2009); the 2s-2p resonance doublets of C IV, N V, O VI, F VII and Ne VIII ions (Elabidi *et al.* 2011). These calculations all use a quantum mechanical approach.

For five lines of Cu I (Zmerli *et al.* 2010) and the lines Ne I 837.8 nm (Christova *et al.* 2010b) and Ar I 737.2 nm (Christova *et al.* 2010a), new Stark broadening parameters are obtained using a semiclassical perturbation approach. A semi-empirical approach, which uses a set of wave functions obtained from Hartree-Fock relativistic calculations and includes core polarization effects, has been applied to 58 lines of Pb IV (Alonso-Medina *et al.* 2010) and 171 lines of Sn III (Alonso-Medina & Colón 2011).

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

34 Pb I (Alonso-Medina 2008), 25 Pb III (Alonso-Medina 2011), 34 Pb IV and 4 Pb V (Bukvić *et al.* 2011), 28 Cd III (Djeniže *et al.* 2009, Bukvić *et al.* 2009b), 13 Si I, 15 Si II, 28 Si III and 9 Si IV (Bukvić *et al.* 2009a), 29 (Bukvić *et al.* 2008) and 19 (Djurović *et al.* 2011) Ar III, 30 Kr III (Ćirišan *et al.* 2011), 12 Ne II, 8 Kr II and 5 Xe II (Peláez *et al.* 2010b), 38 Xe II (Peláez *et al.* 2009a, Peláez *et al.* 2009b), 10 Xe III (Peláez *et al.* 2009b), 5 Au I and 26 Au II (Djeniže 2009), 9 Sb III (Djeniže 2008), 15 Mn I and 10 Fe I (Zielinska *et al.* 2010), 21 Fe II (Aragón *et al.* 2011) and C I 833.5 nm (Bartecka *et al.* 2011).

The regularities and systematic trends of Stark broadening parameters and reasons for deviations have been investigated within the multiplets (Peláez *et al.* 2010b, Peláez *et al.* 2009a), along the homologous sequence of singly-ionized noble gases (Peláez *et al.* 2010a), within the spectral series (Christova *et al.* 2010a) and along isoelectronic sequences (Elabidi *et al.* 2009, Elabidi *et al.* 2011). Also the dependence of electron- and proton-impact Stark widths on the upper-level ionization potential within different series of spectral lines of neutral magnesium (Tapalaga *et al.* 2011) and as a function of charge on the atomic core (Elabidi & Sahal-Bréchet 2011) have been evaluated and discussed. This kind of trend and regularity analysis can be useful for the prediction of Stark broadening parameters and therefore for the spectroscopic diagnostic of astrophysical plasmas.

4.3. Transitions in hydrogenic and helium-like systems

Stark-broadened line profiles of the hydrogen Brackett series have been computed within the Model Microfield Method for the conditions of stellar atmospheres and circumstellar envelopes (Stéhle & Fouquet 2010), and Tremblay & Bergeron (2009) have performed improved calculations for the Stark broadening of hydrogen lines in dense plasmas typical of white-dwarf atmospheres. The central asymmetry of the H β line has been measured and analysed (Djurović *et al.* 2009) and new experimental results for H α and H γ have been published (Mijatović *et al.* 2010a, Mijatović *et al.* 2010b).

Omar (2010, 2011) published new calculations for the Stark broadening of the He I lines at 504.8 nm, 388.9 nm, 318.8 nm, 667.8 nm and 501.6 nm formed in a dense plasma. Tables of Stark broadening for the He I 447.1 nm line have been generated using computer simulations (Gigosos & González 2009). This line and its forbidden component have also been studied theoretically (González *et al.* 2011) and experimentally (Ivković *et al.* 2010, González *et al.* 2011). Gao *et al.* (2008) have carried out experiments for the He I 388.9 nm and 706.5 nm lines.

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. Here the experimental and theoretical 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.

Since the last report an important book has been published (Hartman *et al.* 2008) that gives a comprehensive review of experimental and theoretical work on collisional effects in molecular spectra. In the following sections the items are labelled by 'E' and 'T' to indicate experimental work and theoretical analysis, respectively.

5.1. *Broadening and shift of atomic lines*

New research has been published in the period 2008-2011 and the transitions studied together with the perturbing atoms or molecules are listed below. The work is theoretical except where indicated by 'E'.

H: line wings of Ly α broadened by H and He (Allard *et al.* 2009a, Allard & Christova 2009); line wings of Ly γ by H⁺ (Allard *et al.* 2009b) and H α by H (Allard *et al.* 2008).

He: self broadening of line 3s³S–2p³P (Allard *et al.* 2009c, Allard *et al.* 2011).

Li: self broadening of resonance line (Reggami *et al.* 2009); resonance line broadened by He (Peach & Whittingham 2009, Peach 2010a, Peach 2010b); 2s-3d transition broadened by Ne and Ar (Rosenberry & Stewart 2011).

Na: resonance line broadened by H (Peach 2010b); lines 3s-3p and 3p-3d broadened by He (Peach & Whittingham 2009, Peach 2010a, Peach 2010b).

K: self broadening of resonance line (Reggami *et al.* 2009) and line wings (Talbi *et al.* 2008).

K, Rb and Cs: self broadening of principal series (E) (Vadla *et al.* 2009).

Rb: 5s-5p D2 line, broadening by He, CH₄, C₂H₆, C₃H₈, n-C₄H₁₀ (E) (Zameroski *et al.* 2011).

Cs: 6s-6p D2 line, broadening by ³He, H₂, HD, D₂, N₂, CH₄, C₂H₆, CF₄ (E) (Pitz *et al.* 2010).

5.2. *Broadening and shift of molecular lines*

Much new data have been published since the last report was prepared. The molecules are listed below with their perturbing atomic or molecular species and are labelled by 'E' and 'T' to indicate experimental work and theoretical analysis, respectively.

H₂-Ar: collision-induced absorption (T) (Tran *et al.* 2011b).

D₂-Kr: collision-induced absorption (E) (Abu-Kharma *et al.* 2010).

HI: lines broadened by N₂ (E) (Domanskaya *et al.* 2011).

HBr: self broadening (E) (Domanskaya *et al.* 2009).

HI and HBr: lines broadened by rare gases (E) (Domanskaya *et al.* 2009).

HDO: lines broadened by CO₂ (T) (Gamache *et al.* 2011).

HCl: lines broadened and shifted by N₂, He, Ar and Xe (E) (Hurtmans *et al.* 2009).

HCN: lines broadened by N₂, O₂ and air (E) (Yang *et al.* 2008).

H₂CO: lines broadened by H₂CO and N₂ (E+T) (Jacquemart *et al.* 2010).

HNO₃: lines broadened by N₂ (T) (Laraia *et al.* 2009).

HO₂: lines broadened by N₂ (E) (Miyano & Tonokura 2011).

H₂O₂: lines broadened by N₂, O₂ and air (E) (Sato *et al.* 2010).

H₂O: lines broadened by H₂ (E) (Krupnov 2010), (T) (Wiesenfeld & Faure 2010); by H₂ and He (E) (Dick *et al.* 2010); by N₂ (E) (Lavrentieva *et al.* 2010; by N₂ and O₂ (T) (Gamache & Laraia 2009); by O₂ (E) (Petrova *et al.* 2011; by H₂O (E) (Lisak *et al.* 2009, Ptashnik & Smith 2010); by H₂O, N₂, O₂ (E+T) (Cazzoli *et al.* 2008, Cazzoli *et al.* 2009, Koshelev 2011); by air (T) (Voronin *et al.* 2010); by CO₂ (T) (Sagawa *et al.* 2009); by H₂, He, N₂, O₂ and CO₂ (E) (Dick *et al.* 2009b); by rare gases (E+T) (Fiadzomor *et al.* 2008).

CH₄: lines broadened by N₂ (T) (Gabard & Boudon 2010); by N₂ and O₂ (E) (Lyulin *et al.* 2009); by CH₄ (E) (Smith *et al.* 2010, Lyulin *et al.* 2011); by CH₄ and N₂ (E) (McRaven *et al.* 2011); by O₂ and air (E) (Martin & Lepère 2009); by air (E) (Smith *et al.* 2009, Smith *et al.* 2011).

C₂H₂: broadened by H₂ (T) (Thibault *et al.* 2011a); by H₂ and D₂ (E+T) (Thibault

et al. 2009); by N₂ (E) (Dhyne *et al.* 2009, Fissiaux *et al.* 2009, Dhyne *et al.* 2010); by C₂H₂ (E) (Li *et al.* 2010, Povey *et al.* 2011, Dhyne *et al.* 2011); by He and Ar (T) (Ivanov & Buzykin 2010); by Ne and Kr (E) (Nguyen *et al.* 2009a).

C₂H₄: lines broadened by C₂H₄ (E) (Flaud *et al.* 2011); by Ar (E+T) (Nguyen *et al.* 2009b).

C₂H₆: lines broadened by N₂ (E) (Blanquet *et al.* 2009); by C₂H₆ and N₂ (E) (Devi *et al.* 2010b, Devi *et al.* 2010c); by O₂ and air (E) (Fissiaux *et al.* 2010).

CH₃Br: lines broadened by N₂ (T) (Boussetta *et al.* 2011); by CH₃Br, N₂ and O₂ (E) (Hoffman & Davies 2009); by CH₃Br (T) (Goméz *et al.* 2010).

CH₃F: lines broadened by CH₃F and He (E) (Koubek *et al.* 2011).

CO: lines broadened by CO, N₂ and O₂ (E) (Koshelev & Markov 2009); by H₂, N₂, O₂, CO, CO₂ and He (E) (Dick *et al.* 2009a).

CO₂: by O₂ (E) (Devi *et al.* 2010a); by CO₂ (E+T) (Predoi-Cross *et al.* 2010, Tran *et al.* 2011a); by CO₂, N₂ and O₂ (E) (Li *et al.* 2008); by air (T) (Hartmann 2009), (E) (Gulidova *et al.* 2010), (E+T) (Lamouroux *et al.* 2010); by He (E) (Deng *et al.* 2009); by air and Ar (E) (Farooq *et al.* 2010).

Cs₂: lines broadened by Cs₂ (E) (Misago *et al.* 2009).

N₂: lines broadened by H₂ (T) (Goméz *et al.* 2011); by N₂ (E+T) (Thibault *et al.* 2011b).

NH₃: lines broadened by H₂ and He (E) (Hanley *et al.* 2009); by He (T) (Dhib 2010); by NH₃ (E) (Aroui *et al.* 2009, Guinet *et al.* 2011); by NH₃ and O₂ (E+T) (Nouri *et al.* 2009).

O₂: lines broadened by O₂ (E) (Lisak *et al.* 2010, Wójtewicz *et al.* 2011); by O₂ and OO isotopologues (E) (Long *et al.* 2011); by O₂ and air (E) (Long *et al.* 2010).

O₂-CO₂: collision-induced absorption (E) (Vangvichith *et al.* 2009).

O₃: lines broadened by air (Drouin & Gamache 2008); by N₂ and air (E+T) (Tran *et al.* 2011c).

OH: lines broadened by N₂, H₂O and Ar (E) (Hwang *et al.* 2008).

OCS lines broadened by N₂, O₂ and OCS (E) (Koshelev & Tret'yakov 2009); by N₂ and O₂ (E) (Galalou *et al.* 2011).

I₂: lines broadened by Ar (E) (Phillips & Perram 2008).

6. Databases

Some useful databases are:

Vienna Atomic Line Database (VALD) of atomic data for 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. It can be found at <http://vald.astro.univie.ac.at/> (Kupka *et al.* 1999).

The database of Robert L. Kurucz comprises atomic line parameters, including line broadening. An update to this database is discussed by Kurucz 2011. (<http://kurucz.harvard.edu>)

CHIANTI database (Dere *et al.* 2009) 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 websites <http://sohowww.nascom.nasa.gov/solarsoft> and <http://www.damtp.cam.ac.uk/user/astro/chianti/>.

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 (<http://basecol.obspm.fr>) contains excitation rate coefficients for ro-vibrational excitation of molecules by electrons, He and H₂ 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, that lists atomic data computed in the Opacity Project; namely LS-coupling energy levels, gf-values and photoionization cross sections for light elements ($Z \leq 26$) of astrophysical interest and

(ii) TIPbase that lists intermediate-coupling energy levels, transition probabilities and electron impact excitation cross sections and rates for astrophysical applications ($Z \leq 28$), computed by the IRON Project.

HITRAN – (High-resolution TRANsmision molecular absorption database) is at <http://www.cfa.harvard.edu/hitran/> (Rothman *et al.* 2009). 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 HITEMP (To access the HITEMP data: ftp to [cfa-ftp.harvard.edu](ftp://cfa-ftp.harvard.edu); user = anonymous; password = e-mail address). It contains data for water, CO₂, 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 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> (Jacquinot-Husson *et al.* 2008).

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 and three bibliographic databases providing references on atomic energy levels and spectra, transition probabilities and spectral line shapes and line broadening.

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-Bréchet 2010).

The European FP7 project will finish at the end of 2012. The virtual Atomic and Molecular Data Centre (VAMDC - <http://www.vamdc.eu/>) is being created with the aim of building an accessible and interoperable e-infrastructure for atomic and molecular data that will upgrade and integrate European (and other) A&M database services (Dubernet *et al.* 2011, Rixon *et al.* 2011).

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