

## LXCat : an open-access, web-based platform for data needed for modeling low temperature plasmas

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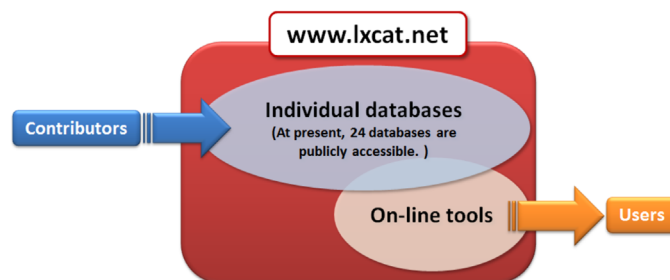
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# LXCat: an Open-Access, Web-Based Platform for Data Needed for Modeling Low Temperature Plasmas

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LXCat is an open-access platform ([www.lxcat.net](http://www.lxcat.net)) for curating data needed for modeling the electron and ion components of technological plasmas. The data types presently supported on LXCat are scattering cross sections and swarm/transport parameters, ion-neutral interaction potentials, and optical oscillator strengths. Twenty-four databases contributed by different groups around the world can be accessed on LXCat. New contributors are welcome; the database contributors retain ownership and are responsible for the contents and maintenance of the individual databases. This article summarizes the present status of the project.



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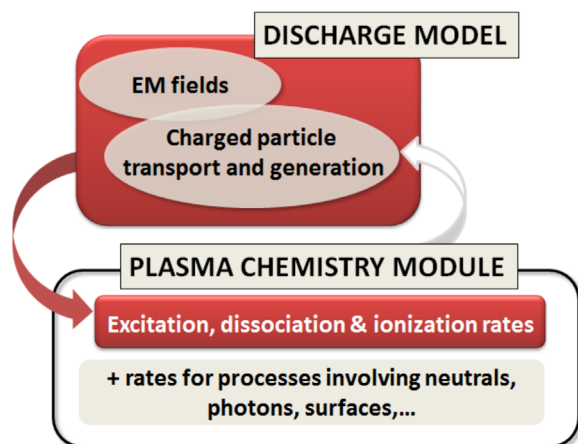
## 1. Introduction

The LXCat platform is an open-access website for storing, exchanging, and manipulating data needed for modeling the electron and ion components of collisional, low-temperature, non-equilibrium plasmas. In such plasmas, the electron mean energy is much higher than the ion mean energy, which is close to or slightly higher than the thermal energy of the background gas. The mobilities of the massive ions are hundreds of times less than those for light electrons, and so the contribution of ions to the electric current is small, except in situations when the ion number densities considerably exceed the electron number density<sup>[1]</sup> (e.g., in sheath regions). The energy gained by the electrons in the electromagnetic fields sustaining the plasma is deposited in the gas in the form of excitation, dissociation, and ionization<sup>[2]</sup>; whereas the energy gained by the ions is mainly converted to gas heating or transferred to the surfaces.<sup>[3]</sup> The properties of low-temperature plasmas depend on the operating

conditions that can be adjusted to optimize production of photons, rich plasma chemistries, or reactive environments near surfaces.

Technologies based on low-temperature plasmas are many.<sup>[4]</sup> To name but a few, these range from mature technologies such as discharge sources of photons for general lighting and gas lasers, to plasma-based technologies for fabrication of semiconductors, treatment of surfaces, deposition of thin films, and more, as well as to the more speculative topics being explored today such as plasma-based therapies for treatment of cancer. Modeling has played an essential role in developing an understanding of the generation and maintenance of the plasmas as well as in guiding the experimental optimization of low-temperature plasma-based devices in different discharge configurations. See, for example, refs.<sup>[5–9]</sup>

Figure 1 illustrates schematically the components of a model of a plasma generated as a result of the application of an external electromagnetic field to a gas. The crux of the model is the upper block, the discharge model, which is



**Figure 1.** Schematic of a discharge model coupled to a plasma chemistry module. The blocks with red background represent sections of the models where data from LXCat can be used.

highly nonlinear because electrons and ions are generated and transported in the space charge fields that they themselves create. The results of this model are the space and time dependent, charged particle concentrations, and the electric field distribution. Depending on the questions being addressed by the model and on the physical conditions of interest, additional modules are added to describe plasma chemistry, radiation transport, surface reactions, gas heating, and hydrodynamics. The lower block in Figure 1 represents a plasma chemistry module. As indicated by the red arrow on the left, the source terms in the plasma chemistry equations are the electron impact excitation, dissociation, and ionization rates, which depend on information from the discharge model. As indicated by the lightly shaded arrow on the right, the presence of excited states and radicals and the degree of ionization does not significantly influence the generation of the plasma unless the relative concentrations of those species are relatively high (greater than approximately  $10^{-5}$ , but depending on exact conditions).

Both the discharge and the plasma chemistry models in Figure 1 require extensive input data, the specific form of which depends on the model formulation. Particle models of the discharge (e.g., kinetic descriptions of electrons and ions) are often used in low-pressure situations and require “complete” sets of cross sections for both electron- and ion-neutral scattering. We will return below to the notion of “completeness.” Fluid models, with separate fluids for each charged particle component, require transport coefficients as input data, and these are averages of cross sections over the energy distribution functions (edf) for electrons or ions. In configurations with high collisionality but low degree of ionization or excitation (i.e., electrons and ions collide mainly with ground state neutrals), the transport data are

usually tabulated as functions of the reduced electric field,  $E/N$ , the ratio of the electric field strength to the neutral density or as functions of the mean electron or mean ion energy. Note that the concept of “electron temperature” applies only to Maxwellian edf’s which are rarely realized in non-equilibrium plasmas. In general, the electron edf is determined by solving a Boltzmann equation using a “complete” set of electron-neutral cross section data as input. The term “complete” is used to imply that the cross sections for all the important electron energy and momentum loss processes are included. Implicit in this definition of completeness is the requirement that the cross section set, when used as input to a Boltzmann solver, yields an electron edf, and hence transport and rate coefficients versus  $E/N$  in good agreement with measurements from swarm experiments. Recall that swarm parameters are transport and rate coefficients, usually measured in homogeneous electric fields and in a background gas with a very low degree of ionization and excitation.<sup>[10]</sup> In many cases, experiments provide transport coefficients to the required accuracy for ions, and transport coefficients in gas mixtures are often approximated by using mixture rules.<sup>[11]</sup> When these are not available, recourse must be made to calculations of cross sections derived from interaction potentials as input<sup>[11]</sup> and from which transport coefficients can be derived.

This article briefly summarizes the internal structure of the LXCat platform and then describes the data types supported by LXCat and available databases, before concluding with a discussion of some practical issues and the current status and future plans for the project.

## 2. Overview of the LXCat Website

The LXCat website is based on a standard LAMP system (Linux, Apache, MySQL, PHP/Python) with an automatic backup. LXCat was designed to be continuously upgradable and users are encouraged to check back regularly for information regarding new features on the site and updates in the data. Access to previous versions of data as they existed at any time after November 2013 is available and earlier versions of the data can be obtained upon request.

An informal forum to share opinions, post doubts and view discussions regarding the content of LXCat is hosted on Google Groups at <http://groups.google.com/forum/#!forum/lxcat>. A guest or visitor can view all the past discussions, as well as use the search facility using relevant keywords. All posts are moderated.

LXCat is structured into individual databases, provided by different contributors, and on-line tools for manipulating the data, as illustrated in the graphical abstract above. General information about the project, detailed list of contributors, quick-start visual instructions, FAQ section,

and a link to scientific publications, and unpublished notes are available on the site. Users are encouraged to make use of these.

The workflow to access data is unified for all types of data. The user is sequentially asked to specify the global data category (electrons and/or ions), choose from the list of active databases, and select species and data types. As a result of the filtering, the list of available data records is shown. At this step, users can choose those records which will be shown more in detail, including the option to download the data in several text (txt, xml) and image formats. It is always possible to return to any previous step and refine search conditions. Graphical representation of data allows simple manipulations specifying the range and the type (linear or logarithmic) of axis. The “complete” set of electron and ion cross sections for several target species can be downloaded at once using a shorter selection process.

The recommended address is [www.lxcats.net](http://www.lxcats.net). The master server has been operational in Toulouse since 2010, and a mirror site was set up at Eindhoven University of Technology in 2013. Daily back-up and usage statistics are provided by LXCat.

### 3. Data Types

The data types that are now supported on the LXCat platform are listed in Table 1 and are described in more detail below.

#### 3.1. Electron Scattering Cross Sections

Both “partial” and “complete” sets of cross sections for electron scattering from individual target species are available on LXCat. A “partial” cross section set for a given target species includes information about only one or a subset of the important scattering processes for that species. The complete sets include a momentum transfer cross section for elastic scattering and total (angle integrated) cross sections for excitation, ionization, attachment processes for a given target species. If the cross section for a particular process is part of a “complete” set, it is so indicated in the comment line for each process. The complete sets in the BSR database (see below) are from *ab initio* calculations. Most of the other complete sets available in the LXCat databases were compiled by individual contributors using partial cross section data from the literature, either measured or calculated, as available. Missing data are estimated and partial cross sections are adjusted within error bars, in order to achieve good agreement between measured swarm parameters and those calculated using the complete set as input to a Boltzmann equation solver. This procedure for determining complete sets of cross sections was pioneered in the 1960's

by Phelps<sup>[12]</sup> and by Crompton<sup>[13]</sup> and their colleagues and is described in the review paper by Petrović et al.<sup>[10]</sup> The determination of a complete set of cross sections consistent with measured swarm parameters and available measurements or calculations of partial cross sections is typical of inverse problems found in many branches of physics. As such, uniqueness is an issue. For this reason, the complete sets reported for the same target species in the LXCat databases often differ in the details.

These cross sections can be downloaded for use in Boltzmann solvers or in Monte Carlo simulations. Or, they can be used directly on the LXCat site for on-line calculations using an abridged version of the two-term Boltzmann solver, BOLSIG+.<sup>[14]</sup> Thus, electron transport and rate coefficients in pure gases or in arbitrary gas mixtures can be obtained directly from the LXCat site when complete sets of cross sections for each of the components in the mixture are available on LXCat. Note that only those datasets flagged as “complete” can be used in the on-line Boltzmann calculations. Note, too, that the common “two-term” approximation used in many Boltzmann solvers does have an influence, slight in most cases, on the calculated transport and rate coefficients. Thus, the type of solver (two-term, multiterm, or Monte Carlo) used in the compilations of swarm-derived cross section sets is stated in the comments for each dataset.

The elastic cross sections in the databases on LXCat are described with a comment line to indicate exactly what is tabulated. These can be total (angle integrated), momentum transfer, viscosity, or effective momentum transfer. The first three are angle-integrated cross sections weighted by the factors, 1,  $(1-\cos\theta)$ , or  $(1-\cos^2\theta)$ , where  $\theta$  is the scattering angle. The effective values include the effects of inelastic collisions as is appropriate for use in the two-term spherical harmonic expansion. See, for example, Baraff and Buchsbaum,<sup>[15]</sup> and Sec. IIB of Pitchford and Phelps.<sup>[16]</sup> Where data are available, the effective momentum transfer cross section is set equal to the sum of the inelastic cross sections plus the elastic momentum transfer cross section. This is an approximate relation.

#### 3.2. Electron Differential Scattering Cross Sections (DCS)

It is usually assumed that elastic momentum transfer and total cross sections for inelastic processes and for ionization provide sufficient information about the angular scattering of electrons for use in homogeneous Boltzmann solvers or Monte Carlo simulations. The accuracy of this assumption has been evaluated in certain gases for calculation of swarm parameters, but because of the lack of full sets of DCS data, very few tests have been made in discharge conditions (e.g., with gradients of fields or densities).<sup>[17]</sup> A set of DCS data for

**Table 1.** Data types available on LXCat and names of databases containing the relevant data.

Species	Data type	Description	Relevant databases on LXCat
Electrons	Scattering cross sections	Total (angle integrated) cross section for inelastic, attachment, and ionization processes. Total, momentum transfer or viscosity cross sections for elastic processes. (Mainly for ground state target species.)	Complete sets: Biagi, Bordage, BSR, CCC, Hayashi, IST-Lisbon, Morgan, Phelps, Puech, SIGLO, TRINITI Partial sets: CCC, Christophorou, COP, Flinders, Itikawa, NGFSRDW, Quantemol
	DCS	Calculated or measured	BSR, CCC, Christophorou
	Oscillator strengths	Measured absolute dipole (optical) oscillator strengths	UBC
	Swarm/transport data	Measured, versus E/N	Christophorou, Dutton, ETHZ, IST-Lisbon, LAPLACE, UNAM
	Rate coefficients	As a function of electron mean energy, or E/N	(under development)
Ions	Interaction potentials	Calculated	Viehland
	Scattering cross sections	Isotropic and backscatter cross sections for noble gas ions in background NG Transport cross sections	Phelps Viehland (under development)
	Swarm/transport data	Measured or calculated versus E/N; analytical formulae	Phelps, UNAM, Viehland

Ion mobilities on LXCat are in cgs units, energies are in eV, and data for all other quantities are reported in mks units.

argon elastic and inelastic scattering is now available in the BSR database on LXCat.

Some limited DCS data from measurements are available for elastic scattering of electrons in SF<sub>6</sub> and CF<sub>3</sub>I in the Christophorou database. Theoretical DCS data for H<sub>2</sub> are available in the CCC database.

### 3.3. Oscillator Strengths

Also available on LXCat are optical oscillator strengths measured using a method known as Dipole (e,e) Spectroscopy<sup>[18]</sup> as briefly described below in the description of the UBC database. Oscillator strength is a quantity that expresses the probability of absorption or emission of electromagnetic radiation in transitions between energy levels of an atom or molecule. These data, combined with a

suitable model such as *BEf* scaling (binary-encounter; oscillator strength,  $f$ )<sup>[19]</sup> can be used to infer the energy dependence and magnitude of electron-neutral scattering cross sections for specific processes for energies greater than several times the threshold energy. These data are included on LXCat because they provide a trove of information about electron-neutral scattering, and in some cases for gases where other scattering data are not available.

### 3.4. Electron Swarm/Transport Data

In addition to the possibility of calculating electron swarm/transport data from complete cross section sets as mentioned above, data from measurements are available on LXCat and are tabulated as functions of E/N. These data include  $\mu N$ , the product of mobility,  $\mu$ , and neutral density,

$N$ ;  $DN$ , the product of the diffusion coefficient (transverse or longitudinal, as indicated) and the neutral density;  $D/\mu$ , characteristic energy; and  $\alpha/N$ , ionization,  $\eta/N$ , attachment or  $(\alpha - \eta)/N$ , net ionization coefficients. All data are reported for room temperature unless otherwise indicated. These data can either be used directly in modeling or can provide valuable spot checks of calculated results. At present, we have excluded swarm data measured in the presence of magnetic fields, where a large body of data exists. This could be included in the future if there is interest.

The drift velocity,  $v_d$ , is the product of  $\mu N$  and  $E/N$  and is the quantity often measured in swarm experiments. For LXCat, experimental values of  $v_d$  were converted to  $\mu N$ , mainly because the dynamic range is smaller and differences between calculation and experiment or between experiments are easier to see at a glance.

### 3.5. Electron Rate Coefficients

Currently, electron collision data are mainly provided as cross sections as a function of electron energy. However, in many practical cases, the “electron temperature,” the mean electron energy or the reduced electric field are the only parameters accessible experimentally (or considered in various plasma models). Many experimental data on electron excitation processes which are being obtained through kinetic analysis of pulsed discharges<sup>[20]</sup> or perturbative measurements (e.g., laser pump-probe technique<sup>[21]</sup>) can only provide rate coefficients as a function of the “electron temperature,” for instance. A new feature being implemented on LXCat will allow uploading data for specific processes directly as rate coefficients. Previously, these processes could only be included as swarm data but they will soon be available for specific products of reactions as well. Such rate coefficients can be compared with other data calculated from corresponding cross sections, using the on-line tools provided by LXCat.

### 3.6. Ion-Neutral Interaction Potentials

A convenient way of storing data quantifying ion-neutral collisions is in the form of interaction potentials, which can be obtained with high precision as a function of internuclear distance from ab initio calculations for simple symmetrical systems. For more complicated systems, potentials are expressed as a function of distance and angle. In principle, DCS can be deduced from the interaction potential, but more commonly, “transport” cross sections are provided (see below) and transport coefficients are expressed in terms of the transport cross sections. The calculations can now be done with sufficient precision that comparisons of theoretical and experimental mobilities

serve as quantitative tests of the accuracy of the interaction potentials.

### 3.7. Ion Scattering Cross Sections

The data presently available on LXCat for ion-neutral scattering are for atomic ions scattering from atoms. The data in the Phelps database were obtained by supposing that the DCS can be approximated as the sum of an isotropic and a backscatter component. These two components were derived for consistency with known information about the DCS and charge exchange cross sections. “Transport” cross sections are provided in the Viehland database, which is presently being updated. These cross sections are calculated from the interaction potentials and are equivalent to the angle averaged DCS's, weighted by the factor  $(1 - \cos^k \theta)$ , where  $k$  identifies the order of the transport cross section.

### 3.8. Ion Swarm/Transport Parameters

Transport parameters (or transport coefficients) for nearly 1000 ion-neutral systems are available on LXCat. Both experimental and theoretical data are available. The theoretical tables give ten transport coefficients as a function of the reduced electric field strength,  $E/N$ . These are the mobility (converted to a reduced mobility  $K_0$  by multiplying by  $P/P_0$  and  $T_0/T$ , where  $P_0$  is exactly 1 bar and where  $T_0$  is 273.15 K), the ion temperatures parallel and perpendicular to the electric field, the ion diffusion coefficients parallel and perpendicular to the field, the skewness of the ion velocity distribution function along the field, the parallel, and perpendicular kurtoses of the distribution, and correlation coefficients between the perpendicular ion energy and the parallel velocity and energy. The gas temperature is indicated in each table.

## 4. Databases

The databases on LXCat are set up and maintained by individual contributors, and the contents remain the responsibility of each contributor. The LXCat support team provides help and guidance on the technical issues. The following paragraphs describe the contents of each of the databases as they existed in May 2016.

References to original sources of data are given in the databases on the LXCat site and more detail is provided below where not available in previous publications.

### 4.1. Biagi-v7.1 and Biagi Databases

These databases contain the complete sets of electron scattering cross transcribed from those available in SF

Biagi's Monte Carlo code, Magboltz.<sup>[22]</sup> The data in Magboltz in its various versions have been continuously updated and improved over the years. The Biagi database contains detailed sets of cross sections for noble gases and for selected molecular gases ( $H_2$ ,  $D_2$ ,  $N_2$ ,  $O_2$ , and  $SF_6$ ) and transcriptions for additional species are planned. This database was previously named Biagi-v8.9 but since the intent of the contributor is to maintain the most recent sets of cross sections in this database, the name has recently been changed to "Biagi." The Biagi-v7.1 database is retained because it includes convenient, simplified representations of data for noble gases as transcribed from version 7.1 of Magboltz.

Since 2012, all upgrades in Magboltz have been derived so that they are not only consistent with measured transport coefficients but also give good fits to the parameters that are important for particle and x-ray interactions such as  $R_o$ , the electron range;  $d\epsilon/dx$ , the energy loss with distance;  $W$ , the energy cost per ion pair versus initial electron energy; and  $F$ , the Fano factor which is the width of the spread of  $W$  values. The upgrades also allow the calculated excitation rates of the levels to be included in a Penning ionization transfer calculation<sup>[23]</sup> of the avalanche gain in gas mixtures used in radiation detectors, but this is not done on LXCat.

There is a complementarity between the radiation measurements and the transport measurements. The cross sections show a dependence on the transport data below 100 eV whereas above 500 eV the cross sections are more sensitive to the radiation parameters.

The recent Magboltz database cross sections are mainly taken from modern accurate experimental electron scattering measurements and only normalized within the allowed experimental error to give best fits to the measured radiation and transport parameters. An example is the vibrational and rotational cross section in molecules where drift velocity measurements in mixtures of the molecular gas with a noble gas allow the accurate normalization of the overall magnitude of the inelastic scattering in the molecule. The accuracy of modern drift velocity data with mixtures of argon, neon and helium allows a normalization of the experimental rotational or vibrational cross sections to typically better than 5%.

The ionization data have been improved in recent years due to the measurements of the Rice University Group<sup>[24]</sup> (see also [http://www.ruf.rice.edu/~atmol/electron\\_data.html](http://www.ruf.rice.edu/~atmol/electron_data.html)) of accurate dissociative ionization in many molecular gases and the charge states in noble gases. The Rice data are consistent with the total ionization measured by Rapp and Englander Golden.<sup>[25]</sup> The consistency between these measurements is within typically 4% and a weighted average is used in the Magboltz datasets. A useful cross check and also some missing ionization data can be supplied by the accurate measurements of Tian and Vidal<sup>[26]</sup> and also Nishimura et al.<sup>[27]</sup>

The effect of fixing the ionization leaves only the excitation cross section as a variable to fit the measured Townsend coefficients. The noble gases have well known level structures and have recently been calculated with good accuracy at threshold by Zatsarinny and Bartschat.<sup>[28]</sup> The threshold cross sections are used in Magboltz and smoothly joined to experimental values at higher energy. The oscillator strengths of many levels have been measured by the British Columbia group<sup>[29]</sup> and use is made in the database of the  $BEf$  scaling<sup>[19]</sup> to obtain cross sections at high energy. The calculated radiation parameters using the  $BEf$  scaling are consistent within 2% of the measured radiation parameters. The cross sections of the non-dipole levels in the noble gases are normalized by an overall scaling factor to give a good fit to the measured Townsend coefficients.

The molecular gases contain additional channels to neutral dissociation that do not exist in the noble gases. The database derives these cross sections from the known oscillator strength distributions from Olney et al.<sup>[29]</sup> and many published measurements of  $\eta$ , the photo-ionization efficiency. The neutral dissociation oscillator strength is equal to the total oscillator strength  $\times (1-\eta)$ . This procedure allows the major part of the neutral dissociation to be calculated using the  $BEf$  formula. The remaining strength to neutral dissociation from non-dipole transitions is typically approximated by two or three levels with a cross section magnitude that is adjusted to fit the Townsend measurements. It should be noted that the triplet dissociation has only a small effect on the radiation parameters because the cross section falls off as  $\epsilon^{-2}$  or  $\epsilon^{-3}$  at energies above 50 eV, where  $\epsilon$  is the electron energy. The molecular radiation parameters thus derived also agree with the experimental values within 2%.

#### 4.2. BOLSIG+ Database

This is a temporary database that is created when requested by the user following execution of the on-line Boltzmann solver. The contents of this database include swarm/transport parameters versus  $E/N$  resulting from the on-line Boltzmann calculations. The data existing in this temporary database can be plotted along with measured quantities available on the other databases or compared with results from other on-line calculations in different gas mixtures. This temporary database is deleted when the user exits the LXCat site.

#### 4.3. Bordage Database

Experimental swarm data in pure gases and in gas mixtures (with argon) were used in an unfolding procedure to derive the complete sets of cross sections for electron



scattering in  $\text{CF}_4$ ,  $\text{CHF}_3$ , and  $\text{Si}(\text{CH}_3)_4$  provided in this database. Cross sections for the dominant processes are tabulated up to electron energies of 500 eV. All the cross sections were derived by using a multiterm solution of the Boltzmann equation in the approximation of the hydrodynamic regime.<sup>[30,31]</sup> The use of these cross sections in the multiterm Boltzmann solver yields drift velocity, ionization and attachment coefficients, diffusion coefficients  $\times N$  (longitudinal and transverse), and characteristic energies, within a few percent of measured values for all gases included in this database. The more common two-term solvers can lead to increasingly large error with increasing  $E/N$  and in cases where cross sections for inelastic processes (vibrational excitation in particular) are large in the region of the Ramsauer minimum. When using these cross sections, it is important to take into account superelastic collisions (using detailed balancing to obtain the cross sections) at low  $E/N$  in order to avoid unphysical results (e.g., the transverse characteristic energy,  $D_T/\mu$ , the ratio of the transverse diffusion coefficient to the mobility, becoming less than the thermal energy of the molecules).

#### 4.4. BSR Database

Angle-integrated and momentum-transfer cross sections for electron collisions with ground-state atoms Be, C, N, F, Ne, Ar, Kr, Xe, as well as DCS data for electron scattering from Ar in the ground state are included in this database. Some selected cross sections for transitions from excited states, as well as for a number of open-shell targets, were added recently, and more uploads are planned in the future. Due to the large amount of data for transitions between excited states, not all these data are available through LXCat. Interested readers should regularly check for updates of the database, and they are also encouraged to contact the authors (O. Zatsarinny and K. Bartschat) directly.

The results in this database are from semi-relativistic (Breit–Pauli) and relativistic (Dirac–Coulomb) close-coupling calculations, in which the resulting equations were solved by the  $B$ -spline  $R$ -matrix (BSR) method, with a fully parallelized and further extended suite of the computer codes published by Zatsarinny.<sup>[32]</sup> An overview of the method and many examples of its application can be found in a recent review by Zatsarinny and Bartschat.<sup>[33]</sup> An important advantage of the method is its ability to employ individually optimized, term-dependent sets of non-orthogonal orbitals to account for the strong term dependence in the one-electron orbitals that is often found in complex targets. Furthermore, recent large-scale calculations, with a dense distribution of pseudostates to account for important coupling to the target continuum via the  $R$ -matrix with pseudo-states (RMPS) approach,<sup>[34]</sup> have

allowed for the ab initio calculation of ionization cross sections.

The BSR predictions have been validated against a number of benchmark experimental data, as well as predictions from other highly sophisticated approaches such as convergent close-coupling (CCC) and time-dependent close-coupling (TDCC) for quasi-1 and quasi-2 electron targets, that is, systems where such results are available. Furthermore, comparisons were made with results from selected other RMPS calculations. Excellent agreement with experiment was achieved in the near-threshold resonance regime, where the excitation process is dominated by negative-ion resonances. Furthermore, extensive convergence checks suggest that the results are also accurate for intermediate energies, that is, for impact energies up to several times the ionization threshold.

Comparisons of measured electron swarm parameters with those calculated using the data sets in this database for noble gases have been reported. These comparisons show that theory has reached the point of being able to provide cross sections consistent with high-precision measurements of swarm parameters in argon<sup>[35]</sup> and neon.<sup>[36]</sup>

#### 4.5. CCC Database

The CCC method is a non-relativistic formulation of the close coupling equations that solves for the scattering  $T$ -matrix in momentum space. The CCC database contains angle-integrated cross sections of electron scattering from atomic hydrogen  $\text{H}^{[37]}$  and helium  $\text{He}^{[38]}$  atoms and the molecular hydrogen ion  $\text{H}_2^+$ .<sup>[39]</sup> For H and He the full sets of cross sections (elastic, momentum-transfer, excitation, and ionization cross sections) are available for scattering from the ground state. The angle-differential cross sections and cross sections for scattering from excited states are available on request from the authors. For  $\text{H}_2^+$  the CCC database provides results from adiabatic-nuclei close-coupling calculations of hot (vibrationally excited)  $\text{H}_2^+$ . Collision data of  $\text{H}_2^+$  and its isotopologues were obtained for scattering from each vibrational state of the electronic ground state and for the distribution of vibrational levels weighted according to the Frank–Condon (FC) factors. In the near future, the CCC database will add comprehensive collision data of electron scattering from molecular hydrogen  $\text{H}_2$ . Presently, the database contains total cross sections and cross sections for elastic scattering and ionization in the energy range from 0.1 to 300 eV and differential cross sections at 17.5 eV for the first seven states of  $\text{H}_2$ .<sup>[40]</sup>

#### 4.6. Christophorou Database

Over the course of many years, IG Christophorou and his colleagues at Oak Ridge National Laboratory and at

National Institute of Standards and Technology (NIST) conducted fundamental investigations of electron interactions with electronegative gases for electrical insulation, plasma processing of semiconductors, and other applications. A subset of this body of work was extracted from the published data tables in references<sup>[41,42]</sup> and uploaded, with permission from the author, to the recently created Christophorou database. For the moment these data include partial sets of electron scattering cross sections in SF<sub>6</sub> and its dissociation products and in CF<sub>3</sub>I, elastic differential cross sections in SF<sub>6</sub> and CF<sub>3</sub>I, and swarm parameters in SF<sub>6</sub>. Further transcriptions of published data by Christophorou and his colleagues to LXCat are in progress.

#### 4.7. COP Database

This database contains the elastic, momentum transfer, and viscosity cross sections for electron scattering from threshold to 1000 eV for argon, krypton, and xenon calculated using our Complex Optical Potential (COP) method based on the relativistic Dirac equations.<sup>[43]</sup> This method allows for flux to escape into the inelastic channels when these are energetically open. As well, charge polarization of the target by the incident electron is included. These inelastic channels include excitation of bound states as well as single ionization of the target atom including ionization of the inner shells. The use of a single method over the whole energy range ensures a consistent dataset for these processes. These results have been published<sup>[44,45]</sup> along with analytic fits to the data. Comparisons with experiments and other calculations show good agreement over the whole energy range.

A notable feature of all these cross sections is the deep Ramsauer minimum below 1 eV incident electron energy. This feature has an important effect on electron transport and diffusion in a plasma environment. It is very difficult to measure cross sections in this region accurately because of the small magnitude and relatively narrow energy spreads of this low energy feature.

These cross sections have been calculated from complex phase shifts obtained with the COP method. Higher order cross sections can be calculated from these phase shifts as well.

#### 4.8. Dutton Database

In 1975, Dutton published a comprehensive survey of electron swarm data available through 1972.<sup>[46]</sup> The data types included in the Dutton review are drift velocity, diffusion coefficients, characteristic energies, excitation coefficients, electron attachment/detachment coefficients, and ionization and recombination coefficients as functions of E/N. Data measured using a wide variety of techniques

were collected, discussed, compared graphically, and selected data were presented in tabular form. Both measured and calculated data were considered in Dutton's survey. At the time of the writing of the Dutton review, several research groups were actively involved in high precision measurements of swarm parameters. High-performance computers were becoming generally available and the analysis of these data allowed the determination of sets of cross sections for electron scattering with ground state neutrals over an energy range from thermal up to some 100 eV.

The Dutton database on LXCat is a transcription of the tabulated experimental data for the following species: He, Ne, Ar, Kr, Xe, N<sub>2</sub>, O<sub>2</sub>, H<sub>2</sub>, CO, CO<sub>2</sub>, and air. The Dutton survey also includes data for NO and NO<sub>2</sub> but these are not yet available on LXCat.

#### 4.9. ETHZ Database

This database contains electron swarm data obtained experimentally using the pulsed Townsend method at the High Voltage Laboratory of ETH Zurich, Switzerland.

A description of the experimental setup can be found in Dahl et al.<sup>[47]</sup> The swarm model and the method for deriving the electron swarm parameters are described in the appendix of Chachereau et al.<sup>[48]</sup> The swarm parameters stored in the database are the net ionization rate coefficient, the electron mobility and the longitudinal electron diffusion coefficient. In the future, ion swarm parameters might be added.

The database presently contains data in pure N<sub>2</sub>, CO<sub>2</sub>, Ar, and mixtures of c-C<sub>4</sub>F<sub>8</sub>O, 2-C<sub>4</sub>F<sub>8</sub>, and HFO1234ze (CF<sub>3</sub>CH=CHF) with these gases. Measurements are currently ongoing and it is planned to expand the database with

1. fluorinated gases and mixtures of those with N<sub>2</sub>, CO<sub>2</sub>, and Ar,
2. mixtures of N<sub>2</sub>, O<sub>2</sub>, CO<sub>2</sub>, and Ar.

#### 4.10. Flinders Database

The Flinders University (Australia) database contains electron-impact excitation integral cross sections (ICSS) for N<sub>2</sub>, NO, CO, CO<sub>2</sub>, and O<sub>2</sub>. Optimized ICSSs for ten electronic states of N<sub>2</sub> were compiled from initial ICSSs derived<sup>[49]</sup> from differential cross section (DCS) measurements.<sup>[50]</sup> Thirty-eight excitation and de-excitation (superelastic) ICSSs for transitions between vibrational levels of the electronic ground state of N<sub>2</sub><sup>[51]</sup> were based on the compilation of Brunger and Buckman,<sup>[52]</sup> extended by a theoretical calculation and a swarm-derived data set.<sup>[53]</sup> ICSSs for

excitation to nine electronic states of NO<sup>[54]</sup> were derived from measurements by Mojarrabi et al.<sup>[55]</sup> and by Brunger et al.<sup>[56]</sup> ICSs for the vibrational excitations (0→1), (0→2), and (0→3) of the ground electronic state of NO were derived<sup>[57]</sup> from measurements in Belgrade.<sup>[58]</sup> Flinders<sup>[59]</sup> and Canberra.<sup>[60]</sup> ICSs for excitation of each of levels 0–7 of the  $A^1\Pi$  state of CO were interpolated from  $BE_f$ -scaled values given in Table 7 of the article by Kato et al.<sup>[61]</sup> The efficacy of those ICSs was based on DCS measurements reported in references.<sup>[61,62]</sup> ICSs for excitation of levels 1–10 of the ground state of CO are as measured by Allan,<sup>[63]</sup> with extrapolation to threshold for level 1.<sup>[64]</sup> Excitation ICSs for three electronic states (including a composite) and levels 1–4 of the electronic ground state of O<sub>2</sub> were derived<sup>[65]</sup> from the recommended values of Brunger et al.<sup>[66]</sup> with the vibrational ICSs extended to threshold with results from Allan.<sup>[67]</sup> Note that this database for the  $a^1\Delta_g$  state,  $b^1\Sigma_g^+$  state and Herzberg pseudo-continuum of composite electronic states in O<sub>2</sub> was largely derived from references.<sup>[68–70]</sup> Excitation ICSs for the Schumann–Runge continuum, Longest band, and Second band of O<sub>2</sub> were determined using  $BE_f$ -scaling by Suzuki et al.<sup>[71]</sup> with the cross section for the Longest band adjusted to match measurements.<sup>[72]</sup> ICSs for elastic scattering and excitation of seven vibrational modes of CO<sub>2</sub> are from a compilation of experimental measurements and theoretical calculations assembled by Campbell et al.<sup>[73]</sup>

#### 4.11. Hayashi Database

Over the course of a long career at Nagoya Institute of Technology and later at the Gaseous Electronics Institute in Nagoya, Professor Hayashi (deceased), and his colleagues determined complete sets of electron scattering cross sections for a large number of target species up to 1 keV. The compilations were assembled giving priority to cross sections measured using electron beam techniques supplemented with analyses from swarm experiments using a two-term Boltzmann solver or Monte Carlo simulations with cross section sets as input.

The Hayashi database on LXCat was constructed by scanning and digitizing curves in reference<sup>[74]</sup> for CF<sub>4</sub>, CH<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>, CCl<sub>2</sub>F<sub>2</sub>, CCl<sub>4</sub>, HCl, H<sub>2</sub>O, SiH<sub>4</sub>, Si<sub>2</sub>H<sub>6</sub>, and SO<sub>2</sub>. The data for Ar and Xe were taken from the tables of recommended cross sections given at the end of the NIFS (National Institute for Fusion Research, Japan) Data Series Reports for Ar<sup>[75]</sup> and Xe.<sup>[76]</sup> The datasets for C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>4</sub>, and CO<sub>2</sub> were digitized by WL Morgan from figures in reference,<sup>[77]</sup> and so these datasets are identical to the ones on the Morgan database. In these references, Hayashi provided extensive bibliographies for his compilations. Finally, the datasets for N<sub>2</sub>O and NO on LXCat were provided by Hayashi to the JILA Atomic Collisions Data Center at the University of Colorado during

WL Morgan's tenure as acting director in 1988–89. Note that the Hayashi database on LXCat presently contains data for 17 neutral species and that Hayashi and his colleagues compiled datasets for other gases as well. See Table 1 in ref.<sup>[77]</sup> for a full list (circa 1990), but not all of these data are readily available.

#### 4.12. IST-Lisbon Database

The IST-LISBON database contains up-to-date electron-neutral scattering cross sections (together with the measured swarm parameters used to validate these data), resulting from the research effort of the Group of Gas Discharges and Gaseous Electronics with IPFN/IST (Instituto de Plasmas e Fusão Nuclear/Instituto Superior Técnico), Lisbon, Portugal.<sup>[78]</sup> The data, compiled from the literature, correspond to contributions from different authors (see detailed references in the database). For each gas the database presents a complete set of cross sections, validated against measured swarm parameters by solving the two-term homogeneous electron Boltzmann equation. In most cases, predictions are in agreement with measurements within 1–20%, for reduced electric fields  $E/N \sim 10^{-4}$ –500 Td. To improve predictions at low  $E/N$ , some sets need to be completed with rotational cross sections,<sup>[79]</sup> also available in the database. Presently, IST-LISBON includes data for Ar, He, N<sub>2</sub>, O<sub>2</sub>, H<sub>2</sub>, and CH<sub>4</sub>. Work is in progress to publish data for CO<sub>2</sub> and CO.

#### 4.13. Itikawa Database

The data available on this database were transcribed from the tables appearing in publications.<sup>[80–85]</sup> Sets of recommended data for total (angle integrated) cross sections are available for electron collisions with H<sub>2</sub>, N<sub>2</sub>, O<sub>2</sub>, CO, H<sub>2</sub>O, and CO<sub>2</sub>. The recommendations are based on available experimental data. In that sense, the present sets of cross sections are not “complete.” After the evaluation of each experiment, uncertainties have been estimated and were presented in each paper.

#### 4.14. LAPLACE Database

This database includes electron swarm data in a number of pure gases and in some gas mixtures appearing in articles published after the Dutton review article.<sup>[46]</sup> This database covers much of the literature, but it does not aim to be exhaustive except for the noble gases. Data appearing here were transcribed from tables when these were available in the publications or were digitized from figures, as indicated in the database. References are listed in the LAPLACE database.

#### 4.15. Morgan Database

For a wide variety of applications and starting in the mid-1970's, WL Morgan compiled the sets of electron scattering cross sections in this database. These are suitable for use with two-term Boltzmann solvers. Complete sets of cross sections for noble gases and common molecular gases are available, certain datasets cover a wider energy range than others, and some are more detailed than others. The cross sections for excitation in the noble gases, for example, include only one or two effective excitation levels which represent well the electron energy loss processes. Details of the cross sections data for Cl<sub>2</sub>, F<sub>2</sub>, HCl, CF<sub>4</sub>, SiH<sub>4</sub>, and CH<sub>4</sub> are provided in review articles.<sup>[86,87]</sup> There is some overlap with datasets in the Phelps and Hayashi databases on LXCat which is retained simply so that users can recover previously used data. The Morgan data compilations were freely available via the website for Kinema Research and Software from the mid-1990's and since 2010 they have been available publically on the LXCat website. These data and Morgan's ELENDF Boltzmann solver<sup>[88]</sup> have been extensively used in the low-temperature plasma community.

Some cross sections for energy loss or ionization processes for electron collisions with radicals or excited states are also included in this database. These are not part of "complete" sets but are useful for calculating rate coefficients for the processes when the radicals are present as minority species and do not influence the electron edf.

One point to note is that the rotational excitation is treated using a continuous approximation for rotation (CAR) that is described by Frost and Phelps<sup>[12]</sup> and by Morgan and Penetrante.<sup>[88]</sup> The value of CAR is given in the datasets but is not used in the on-line Boltzmann solver. Thus, caution should be exercised in the interpretation of the on-line calculations of swarm parameters at low E/N where rotational excitation/deexcitation can have an influence.

#### 4.16. NGFSRDW Database

This dataset consists of excitation cross sections for transitions in certain noble gases (NG) between fine-structure (FS) levels including excitations from both the ground state and excited states for argon and krypton neutral atoms. These were calculated using the Relativistic Distorted Wave (RDW) method as originally described by Zuo et al.<sup>[89]</sup> (The database name comes from the three acronyms defined here.) In this method, the initial and final levels are represented by relativistic configuration-interaction Dirac-Fock wave functions, which provide unique wave functions and energies for each FS level. The RDW method is a relativistic version of the distorted-wave Born approximation including full exchange. The database uses

the Paschen notation to designate the various levels included.

These cross sections are reasonably accurate except near threshold and the behavior is governed by the total (orbital plus spin) angular momentum *J* of the initial and final states. Since the total angular momentum varies among the various FS levels in a given manifold, the cross sections have differing high-energy behavior depending on *J*.

The cross sections for argon have appeared as: ground to the 4 p manifold,<sup>[90]</sup> to the 3 d, 5 s and 5 p manifolds,<sup>[91]</sup> from the metastable levels of the 4 s manifold to the 5 p manifold,<sup>[92]</sup> from the resonance levels of the 4 s manifold to the 4 p manifold as well as transitions among the FS levels of the 4 s and 4 p manifolds.<sup>[93]</sup>

For krypton, the cross sections have been published as follows: from the ground state to the 5 s manifold,<sup>[94]</sup> to the 4 d, 5 p, and 6 s manifolds<sup>[95]</sup> and to the 6 p manifold<sup>[96]</sup>; from the 5 s metastable levels to the 5 s and 5 p manifolds<sup>[97]</sup>; from the 5 s manifold to the 6 p manifold.<sup>[96]</sup>

These cross sections have been incorporated into a collisional-radiative model for low temperature plasmas.<sup>[93,96]</sup> Similar data for other transitions can be provided upon request.

#### 4.17. Phelps Databases

For many years and in response to many queries, AV Phelps (deceased) made his data compilations available freely through an ftp site hosted by JILA at the University of Colorado ([jila.colorado.edu/~avp/collision\\_data/](http://jila.colorado.edu/~avp/collision_data/)). At this writing, Phelps' ftp site is still on-line and the data files are quite useful for their many comments, references, etc. A part of these data (electron scattering cross sections, ion scattering cross sections, and ion swarm data) were uploaded to LXCat in 2010.

The electron-neutral scattering cross sections are compilations of "complete" sets of data resulting from analyses of measurements of swarm parameters using a two-term Boltzmann code. In most cases, these cross sections were assembled in the 1970's and 1980's. In only a few cases have they been modified or tested since that time. "Complete" sets of electron-neutral cross sections from the original Phelps website for Ar, CO, CO<sub>2</sub>, H<sub>2</sub>, He, Mg, N<sub>2</sub>, Na, Ne, NO, O<sub>2</sub>, and SF<sub>6</sub> are on LXCat. These cross sections were derived to give a good fit to published electron transport, excitation coefficient, attachment coefficient, and ionization coefficient data for the pure gases. In many cases, they have been tested satisfactorily against similar swarm data for gas mixtures, for example, CO<sub>2</sub> laser mixtures, H<sub>2</sub>-Ar mixtures, N<sub>2</sub>-SF<sub>6</sub> mixtures, and atmospheric pressure dry and moist air. In several cases, for example, He, Ar, and Xe, no attempt was made to distinguish among the various excited states and find the cross sections satisfactory for models of

mixtures and of ionization and transport in the pure gases. Rather, a global cross section intending to represent well all excitation processes is provided.

A dataset for H<sub>2</sub>O is also available; however, in the Phelps analysis rotational excitation/deexcitation was treated using the CAR approximation for rotational excitation/deexcitation as described above for the Morgan database. Since H<sub>2</sub>O has a large dipole moment, rotational excitation/deexcitation processes are very important for low energy electrons and so the cross sections in this database should be used with caution or a treatment of rotational excitation/deexcitation should be added.

The cross sections for ion-neutral scattering in the Phelps database are for elastic scattering and suppose that the DCS can be modeled as the sum of isotropic and backscatter components (in the center of mass). These two components are given for Ar<sup>+</sup> in Ar, He<sup>+</sup> in He, and Xe<sup>+</sup> in Xe as is the isotropic component for Xe<sup>+</sup> in Ne.

Some ion swarm data (ion mobility, characteristic energy and ion temperature) are given in this database for Ar<sup>+</sup>, He<sup>+</sup>, N<sub>2</sub><sup>+</sup>, and Ne<sup>+</sup> in their parent gas and for N<sup>+</sup> in N<sub>2</sub>. Some of the data are tabulated and others are fits to analytical formulae.

#### 4.18. Puech Database

Complete sets of electron scattering cross sections in Ar, C<sub>2</sub>H<sub>4</sub>, C<sub>3</sub>H<sub>6</sub>, Ne, and in Xe were assembled by V Puech<sup>[98–100]</sup> and his colleagues at LPGP in Orsay, France starting in the 1980's. These include the first attempts to assemble detailed sets of cross sections for noble gases from beam measurements and/or theory. In all cases, some modifications or extensions of the literature values were needed to obtain consistency with swarm parameters. Calculations of swarm parameters were made using a two-term Boltzmann solver as well as the multiterm solver developed by Ségur and Bordage.<sup>[31]</sup>

#### 4.19. Quantemol Database

Quantemol Ltd (<http://www.quantemol.com>) has developed an expert system, Quantemol-N,<sup>[101]</sup> which runs *R*-matrix codes.<sup>[102,103]</sup> Besides performing low-energy electron-molecule collision calculations using the *R*-matrix method this code also includes a number of other facilities such as the calculation of electron impact ionization cross sections using the binary encounter Born (BEB) method of Kim and Rudd.<sup>[104]</sup> Quantemol has provided a variety of electron collision data for LXCat. Below the species that have been studied are listed; we note that in most cases the results have not been formally published.

Species for which electron impact ionization data are provided include BF<sub>3</sub>, C<sub>2</sub>, C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>2</sub><sup>+</sup>, C<sub>2</sub>OH<sub>6</sub>, C<sub>3</sub>, C<sub>3</sub>H<sub>4</sub>, C<sub>3</sub>N,

CaF, CaF<sup>+</sup>, CF, CF<sub>2</sub>, CF<sub>4</sub>, CH, CH<sup>+</sup>, CNH, CO, CO<sub>2</sub>, CO<sub>2</sub><sup>+</sup>, CONH<sub>3</sub>, COS, CS, F<sub>2</sub>O, H<sub>2</sub>, H<sub>2</sub><sup>+</sup>, H<sub>2</sub>O, H<sub>2</sub>S, HBr, HCHO, HCN, HCP, Kr, N<sub>2</sub>, N<sub>2</sub>O, NH<sub>3</sub>, NO<sub>2</sub>, O<sub>2</sub>, O<sub>3</sub>, PH<sub>3</sub>, SiF<sub>2</sub>, SiH<sub>4</sub>, SiO, and SO<sub>2</sub>. In addition for methane<sup>[105]</sup> elastic total cross sections are also provided.

#### 4.20. SIGLO Database

The SIGLO database is the “in-house” data for electron-neutral scattering cross section sets used by the group GREPHE at LAPLACE in Toulouse. For the most part these data are complete sets and have been taken from the references listed in the database for each neutral species. Some of the data sets were originally compiled by AV Phelps or by WL Morgan and so are essentially duplicates of the data existing in other databases on the LXCat site. The duplication is retained for consistency with the older, pre-LXCat data file (siglo.sec) which was distributed, along with a file of references with the freeware Boltzmann solvers, BOLSIG<sup>[106]</sup> and BOLSIG+.<sup>[14]</sup> This database has been updated at irregular intervals as is documented on the LXCat site, and previous versions can be accessed through LXCat.

#### 4.21. TRINITY Database

An extensive database for electron scattering cross sections for a number of species is available in the database for “EEDF,” a freeware Boltzmann solver based on the two-term approximation that can be downloaded through the LXCat site.<sup>[107]</sup> So far, the only data from “EEDF” that have been transcribed to the TRINITY database on LXCat are those for O<sub>2</sub>. Considerably, more data are available through “EEDF.” These include complete sets for the following species: He, Ne, Ne\_reduced, Ar, Kr, Xe, Xe\_reduced, Cs, Na, O, H<sub>2</sub>, N<sub>2</sub>, O<sub>2</sub>, CO, F<sub>2</sub>, HCl, CO<sub>2</sub>, H<sub>2</sub>O, BCl<sub>3</sub>, NF<sub>3</sub>, CF<sub>3</sub>I, CF<sub>4</sub>, CH<sub>4</sub>, C<sub>2</sub>H<sub>4</sub>, SF<sub>6</sub>. Work is in progress to transcribe more of these data to the TRINITY database on LXCat site.

As a rule, the data compilations in “EEDF” have been verified by comparison of calculated and measured electron transport and kinetic coefficients over a wide range of reduced electric field, *E/N*, values. The data in “EEDF” are freely available and can be used in other numerical codes. Using the “EEDF” package, the data can be selected for graphical display and saved in two-column tables with electron energy in eV and electron scattering cross section in units of 10<sup>-16</sup> cm<sup>2</sup>.

It is important to note that the “rotational cross section” for O<sub>2</sub> (available through LXCat) should not be considered as corresponding to an individual process. Rather, it is specific to the treatment used in “EEDF” which describes the multiple excitation/deexcitation processes in electron collisions with molecules having a thermal rotational

distribution. A compact form of the collision operator for these conditions was derived in references,<sup>[108,109]</sup> and a similar expression was recently derived by Ridenti et al.<sup>[79]</sup> Similarly, the rotational cross sections in the “EEDF” data bank for H<sub>2</sub>, N<sub>2</sub>, and CO (soon to be available through LXCat) should only be used when rotational processes are treated in the same way as in the “EEDF” package. See the Technical Note by AP Napartovich et al on the LXCat site <http://www.lxcat.net/notes/> for details.

#### 4.22. UBC Database

The UBC database consists of Absolute Dipole (Optical) Oscillator Strengths as a function of photon energy for 65 neutral atoms and molecules for photoabsorption in the vacuum UV and soft X-ray regions of the electromagnetic spectrum. The data were obtained in both the discrete and continuum regions by fast electron scattering using electron energy loss spectroscopy (EELS) at zero degrees scattering angle. This method, known as Dipole (e,e) Spectroscopy, involves Bethe–Born conversion of the electron scattering intensities and Sum–Rule normalization to give absolute scales. The technique utilizes the virtual photon field created by a fast electron scattered in the forward direction (i.e., at negligible momentum transfer). Under these conditions the electron energy loss is equivalent to the photon energy and the method gives results entirely equivalent to those that could be obtained using continuum light sources such as monochromated synchrotron radiation. It is important to note that these data do not suffer from the line saturation effects (linewidth–bandwidth interactions) which can cause large errors in optically determined oscillator strengths for discrete transitions with narrow natural linewidths. The experimental methods, data processing and some corrections to earlier data are presented in Chan et al.<sup>[18]</sup>, Chan et al.<sup>[110]</sup>, and Olney et al.<sup>[29]</sup> Both “low” (typically 1.0 eV fwhm) and “high” (typically 0.048 eV fwhm) resolution data are tabulated and can be plotted. These data are derived from a series of measurements made by Professor Chris Brion and his group at the University of British Columbia (UBC) between 1991 and 2002. References to their publications are given in the UBC database for each neutral species and should be included in all publications making use of these data. Occasionally, the tabulated values of oscillator strength are negative below and close to threshold for inelastic scattering. This simply reflects the statistical accuracy of the data.

#### 4.23. UNAM Database

The UNAM database<sup>[111–113]</sup> was originally named the “Urquijo” database. It contains measured and calculated

electron and ion swarm coefficients for a wide range of gases and gas mixtures. The set of density-normalized swarm coefficients, given as a function of E/N comprises ionization ( $\alpha/N$ ), attachment ( $\eta/N$ ), effective ionization ( $\alpha - \eta/N$ ), longitudinal diffusion ( $ND_L$ ), electron mobility times gas density product ( $\mu N$ ), and ion reduced mobility ( $K_0$ ), (binary or ternary) ion–molecule reaction rates and electron detachment ( $\delta/N$ ). This tabulated set of swarm data comprises electron and ion interactions with the noble gases (He, Ne, Ar, Xe), atmospheric gases (O<sub>2</sub>, N<sub>2</sub>, H<sub>2</sub>O, N<sub>2</sub>O, CO<sub>2</sub>), hydrocarbons (CH<sub>4</sub>), fluororocarbons (CF<sub>4</sub>, C<sub>2</sub>F<sub>6</sub>, CHF<sub>3</sub>, CF<sub>3</sub>I, C<sub>4</sub>F<sub>8</sub> and C<sub>2</sub>H<sub>2</sub>F<sub>4</sub>), and SF<sub>6</sub>. Recent research on molecules of biological interest such as Tetrahydrofuran (THF, C<sub>4</sub>H<sub>8</sub>O) and Tetrahydrofurfuol Alcohol, (THFA, C<sub>5</sub>H<sub>10</sub>O<sub>2</sub>), as well as electron and ion swarm data in binary mixtures of H<sub>2</sub>O with other gases will soon be available in this database.

#### 4.24. Viehland Database

A large selection of interaction potentials for atomic ion–atoms systems is available in the Viehland database. The newer ones were obtained ab initio using: CCSD(T) or higher levels of theory; large basis sets (such as aug-cc-pV5Z) for small atoms and small-core relativistic effective core potentials for large atoms; inclusion of spin-orbit interaction effects; full counterpoise corrections at each ion–neutral separation to correct for basis set superposition error; and extrapolation to the complete basis set limit.<sup>[114]</sup> The ab initio calculations were made by specifying a high level of accuracy for the convergence of numerical integrals and for evaluation of the total energies. Special care was taken to be sure that the potentials smoothly joined the polarization potentials that are known to be correct at very large separation. The calculations are carried out at small enough separation that the repulsive region (positive potential energies) is probed.

From the tabulated potentials it is possible to make classical-mechanical calculations<sup>[115]</sup> of as many as 30 transport cross sections, the first and second being the momentum-transfer (or diffusion) and viscosity cross sections. When the potentials obey the requirements listed above, it is possible to obtain cross sections accurate to 0.04% or better over wide ranges of the ion–neutral collision energy, typically 10<sup>−9</sup> to 10 hartree (1 hartree = 27.211 eV).

As indicated in reference,<sup>[115]</sup> the Fortran computer program named PC that performs such calculations is available upon request; we intend to add this program to LXCat in the near future. For atomic ions interacting with their parent gases, semi-classical techniques may be used to take resonant charge transfer into account. A Fortran computer program named QEx is available<sup>[116]</sup> for making such calculations from g-u pairs of interaction potentials.

Calculating quantum-mechanical cross sections from scattering phase shifts is possible,<sup>[117]</sup> but this is necessary only for extremely light ions and gases, and even then only when the energies probed correspond to gas temperatures below a few K and electric field strengths that are almost zero.

There are two main types of gaseous ion transport data (swarm/transport parameters) in this database. The experimental tables include all of the smoothed and critically assessed data contained in four papers published in Atomic and Nuclear Data Tables.<sup>[118–121]</sup> They also include data published since the last of these papers. Since the goal is to be complete, some of the data contained here replicates data contained in other sections of the LXCat database.

The theoretical tables include results calculated from the high-quality, ab initio ion-neutral interaction potentials discussed above. These calculations are based on the Gram-Charlier method<sup>[122,123]</sup> for solving the Boltzmann equation for ions in a series of successive approximations. The accuracy of the results varies, as indicated in each table, but for atomic ion-atom systems they are always more accurate than can be obtained experimentally. Ordinarily, there are six tables for each ion-neutral combination – five cover wide ranges of E/N for gas temperatures of 100, 200, 300, 400, and 500 K, while the sixth gives the zero-field mobility and diffusion coefficients as a function of temperature. For ions moving through helium, there are also tables for 4.35 K. Tables for other gas temperatures are given in situations where there are experimental data at those temperatures.

## 5. Concluding Remarks

Several guidelines were defined at the beginning of the LXCat project. These are: (1) anyone willing to contribute data to the site can request a password and set up a database; the contents and maintenance of the databases remain the responsibility of the individual contributors. (2) The site is open access and data can be downloaded without registering or paying a fee. (3) The databases are dynamic and contributors are free to make changes as they see fit.

One consequence of the first guideline is that data for the same processes can be listed in multiple databases. While LXCat does not provide a recommendation, an informal effort to publish documentation and intercomparisons of data on LXCat was initiated in the context of the GEC (Gaseous Electronics Conference) Plasma Data Exchange project. To this end, three papers<sup>[35,36,124]</sup> appeared in 2013 documenting the electron-noble gas scattering cross sections available at that time on LXCat, along with an article about computational techniques for calculating cross sections in atomic systems.<sup>[125]</sup> Intercomparisons of cross section data and comparisons of experimental and

calculated swarm parameters using these data were made. While not going so far as to recommend data, these papers provide guidance as to which data users should select for a given situation. A second series of papers documenting data in H<sub>2</sub>/D<sub>2</sub>, in N<sub>2</sub>, and in O<sub>2</sub> is in progress. The LXCat team is pursuing further work in this direction and efforts on the part of other people in the community to critically review data on LXCat are welcome.

The second guideline – open access – should not mean that downloaded data become anonymous. Proper referencing of data downloaded from the site is essential for the survival of LXCat, and publications making use of data downloaded from LXCat should reference the site as well as the publications, if any, listed in each contributor's database. The format for referencing data retrieved from the site is: [database name], www.lxcat.net, [retrieved date]. It is hoped that members of the scientific community remain vigilant about the need for proper referencing of downloaded data. LXCat does not grant authorization to third parties (commercial interests, in particular) to download and distribute data from the LXCat site. Third parties are requested to contact LXCat for an explicit policy statement on this point.

Thirdly, the databases on LXCat are dynamic; that is, rather than assign a DOI to each database (which would become immutable), contributors are allowed to upgrade their database as new data become available or when corrections are needed. The history of changes in each database is recorded on the site, and data as they existed at any date after November 2013 can be recovered on-line. Versions predating November 2013 are available upon request. All downloaded files include the retrieved date in the header text, and, for traceability of data used in calculations, it is important to include this date in all references to data downloaded from the site.

The format of data downloaded from LXCat is compatible with an increasing number of codes, both freeware and commercial, and links to some are listed on the website. In addition, LXCat is set up to act as a node for VAMDC, the Virtual Atomic and Molecular Data Center, which is a portal through which a number of databases can be accessed.<sup>[126]</sup> While many of the data available through VAMDC are relevant to needs for astrophysics, VAMDC is not limited to this topical area and all LXCat database contributors have the option of having their data indexed for VAMDC. However, only those data flagged with “VAMDC” can be seen through this portal. LXCat welcomes opportunities for linking to or collaborating with other projects.

It is worth mentioning at this point that discussions have been initiated in the low temperature plasma community about developing databases and service similar to LXCat but for low and high pressure plasma chemistries. Such datasets usually consist of rate coefficients for two and three body processes. LXCat is being extended to

accommodate this data type for electrons and ions. Both for LXCat and such new databases, discussions remain open about the strategies and requirements for validating complete datasets of cross sections/rate coefficients for given plasma systems.

It is clear that the wish of the community is going toward “validated” datasets of cross sections (+rate coefficients) to be readily available for plasma modeling. However as stressed in the introduction and again several times in the description of data available in databases, the completeness of a dataset cannot be defined generally. This is a specific issue related to the nature itself of low temperature plasmas where the properties of the system cannot be easily parameterized as a function of a few parameters like pressure, temperature and gas composition like in thermal systems. For going beyond the “cold plasma limit” (i.e., negligible densities of excited state densities who play then no role into electron and ions dynamics), it is necessary to take into account the population densities of excited states explicitly and include their individual contributions. To do so, it is then necessary to go for state-to-state excitation kinetics. Many efforts are still needed into that field but the aim of LXCat is gathering available data for electrons and ions and to provide tools to users to assess such data. For the validation of given datasets, discussions are currently ongoing in the plasma community for the strategies and methods to be developed and adopted to attain such a goal.

Since the beginning of the project, more than 40 people representing institutions in 15 different countries have devoted time and effort to the LXCat project. The contributors include modeling groups who are willing to make their collections of data available publically as well as experimental or computational groups who generate data. The data contributors and the other people who have contributed to the infrastructure of the site itself constitute the “LXCat team,” most of whom are co-authors on this paper. Usage statistics indicate a steady increase in the number of visitors from around the world, and a glance at the titles of papers referring to LXCat show that researchers from many different scientific and technical areas make use of the data available on this site. The website has undergone a complete transformation since the first public version in 2010<sup>[127]</sup>; ion and electron data have been merged into a common structure that can be upgraded for the foreseeable future. Regular backups of the databases are made and so the data themselves are quite secure. Nevertheless, survivability of the overall project has been a concern because there has been no well-defined structure and very little funding. To these ends, the non-profit organization “Data for Modeling Plasmas” was set up in 2015 which defines a structure and provides a means for continuity and for accepting donations, annual dues, or grants from individuals or institutional partners. The objective of this organization as stated in its formal by-laws is “to facilitate

the exchange of numerical tools and data for modeling the physics and chemistry of plasmas.” Further information can be found at <http://assoc.lxc.net>. LXCat is a community-wide project, and its long-term future depends on the contributors’ maintaining and updating their databases and on the user community’s help in maintaining the visibility of the project.

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