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LiDB: Database of atomic radiative lifetimes for plasma processes

Alec Owens [a], Tingting Chen [a], Christian Hill [b], Sebastian Mohr [c], Jonathan Tennyson [a,*]

[a] Department of Physics and Astronomy, University College London, WC1E 6BT, London, United Kingdom
[b] Atomic and Molecular Data Unit, Division of Physical and Chemical Sciences, International Atomic Energy Agency, Vienna, Austria
[c] Quantemol Ltd., 320 City Rd London EC1V 2NZ, United Kingdom

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ABSTRACT

LiDB is a database of molecular radiative lifetimes (Owens et al., 2023), created to aid in the modelling of radiative effects in low-temperature plasmas. Here, we report the addition of atomic radiative lifetimes to LiDB. Datasets are generated for neutral and singly-charged atomic species based on energy levels, transitions, and transition probabilities extracted from the National Institute of Standards and Technology (NIST) Atomic Spectra Database (ASD). The main data output of LiDB is radiative lifetimes of atomic states defined uniquely by atomic term symbols and electronic configurations. The effects of the total angular momentum quantum number J on the lifetimes are averaged over using an atomic state lumping procedure. LiDB also provides partial lifetimes which yield information on the dominant radiative decay channels from each state. Datasets are available for 35 neutral and 19 singly-charged atoms with new species to be added in the future. LiDB is freely available at www.exomol.com/lidb where users can dynamically view atomic and molecular datasets or use an application programming interface (API) to request data.

1. Introduction

Radiative decay processes are an inherent part of low-temperature plasmas (and plasmas in general). It is common to find atoms and molecules in excited states emitting radiation through a variety of emission pathways and on different timescales. These emissions complicate diagnostic measurements and lead to a range of effects, from altering the energy and temperature distribution within the plasma to radiation-induced damage. For example, ultraviolet (UV) emissions from the plasma used for etching and deposition in semiconductor manufacturing can damage the underlying substrate [1].

Modelling radiative effects in plasmas requires a detailed understanding of the constituent atomic and molecular species. The radiative lifetime of an atomic or molecular state, determined from the transition probabilities linking that state with all possible states lower in energy, encapsulates the radiative behaviour. Undertaking full collisional-radiative modelling of technological plasmas would be a considerable achievement [2,3] and doing so requires high-quality input data, the importance of which is being increasingly recognized in the simulation of low-temperature plasmas [4]. It is common practice for plasma models to ignore the role of radiation, simply because accurate and comprehensive data on radiative lifetimes and emission channels are lacking. As a result, low-pressure plasma processes cannot be fully understood or rigorously optimized.

Previously, we developed and deployed a new database of molecular radiative lifetimes called LiDB [5], hosted at www.exomol.com/lidb. Total lifetimes of molecular states with full quantum number assignment were derived and compiled at vibrational-state resolution from comprehensive molecular line lists (extensive compilations of energy levels and all possible transitions between them with associated Einstein A coefficients) from the ExoMol database [6–9]. ExoMol is a spectroscopic database aiding studies of exoplanets, cool stars and other astronomical objects, as well as a variety of terrestrial applications. Also provided in LiDB were partial lifetimes of up to five of the most dominant decay channels per molecular state, allowing users to establish the primary emission pathways occurring in a species. A total of 36 molecules composed of up to four atoms were added to LiDB. LiDB lifetimes are currently being integrated into the Quantemol database (QDB) of plasma chemistries and reactions [10], which provides cross sections and rates of processes important for plasma models involving heavy particle collisions (chemical reactions) and electron collision processes.

In this work, we report the addition of atomic radiative lifetimes to LiDB. Total lifetimes and partial lifetimes of neutral and singly-charged atomic species are produced from energy levels, transitions, and Einstein A coefficients extracted from the National Institute of Standards and Technology (NIST) Atomic Spectra Database (ASD) [11].

* Corresponding author.
E-mail address: j.tennyson@ucl.ac.uk (J. Tennyson).

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NIST ASD is a comprehensive resource for atomic spectroscopy, offering critically evaluated and internally consistent data on atomic energy levels, transition wavenumbers and probabilities, and many more key spectroscopic parameters. The database is continually updated and is an indispensable reference for scientific and industrial applications concerning atoms. The NIST ASD has performed countless critical compilations and evaluations of atomic transition data. The reader is encouraged to seek further details on the history and development of NIST ASD in Refs. [12,13] and on its website at www.nist.gov/pml/atomic-spectra-database. There is a wealth of spectroscopic information in the NIST ASD which LiDB aims to simplify so that users can incorporate lifetime data into their plasma models.

The paper is structured as follows: In Section 2 we describe the methodology used to produce total lifetimes and partial lifetimes of atomic states. An overview of the LiDB database is given in Section 3, before concluding remarks are offered in Section 4.

2. Methodology

2.1. Atomic spectroscopic notation

LiDB utilizes the same atomic spectroscopic notation utilized by the NIST ASD for each species. A detailed description of atomic structure, terminology and notation is provided in Ref. [14] and on the website of NIST ASD. States in LiDB were defined and parsed using PyValem format [15,16], which is a Python package designed for specifying the species and states of atoms and molecules in a standardized way.

In LiDB, atomic states are defined by an electronic configuration and an atomic term symbol. Atomic configurations, which describe the arrangement of the electrons, are defined by the principal quantum number n, the orbital angular momentum quantum number l (represented by the letters $s, p, d, f, \ldots$ for values of $l = 0, 1, 2, 3, \ldots$), and the number of electrons in each subshell.

Most atoms contained in LiDB are light (possess a low atomic number) and their term symbol is defined within the LS coupling scheme (also known as Russell-Sanders coupling). In LS coupling, atomic terms are labelled as ${}^{2S+1}L$ using the total spin quantum number S, and the total orbital angular momentum quantum number L (denoted by capital letters $S, P, D, F, \ldots$ for $L = 0, 1, 2, 3, \ldots$). Odd parity states have a superscript parity label ° appended to the atomic term while even parity states have no parity superscript label. The spectra of more complex atoms (Fe, Cr, Mn, Ti, V), due to their congested nature, possess atomic term symbols that are prefixed with a lower-case letter ($a, b, c, x, y, z, \ldots$) to differentiate the various states. Atomic term symbols of the noble gas neutral atoms (Ne, Ar, Kr, Xe) are labelled using Racah notation [14], where terms have the form $nl[K]_J$. Here, K is an intermediate angular momentum quantum number based on the sum of the core and excited electron quantum numbers (depending on the coupling scheme).

2.2. Procedure used to generate lifetimes

For an atomic state, the radiative lifetime τ_i (in seconds) is defined as,

$$\tau_i = \frac{1}{\sum_f A_{if}}, \tag{1}$$

and is calculated by summing up all the Einstein A coefficients A_{if} (in seconds^{-1}) from an initial state i to any connected final state f that has a lower energy.

In the NIST ASD, atomic energy levels are assigned an atomic term symbol, electronic configuration, and total angular momentum quantum number J. Plasma modelling is not usually at a resolution that requires lifetimes of atomic states resolved over the J quantum number. Therefore we develop an atomic state "lumping" procedure to produce J-unresolved radiative lifetimes and states in LiDB. A similar state lumping procedure was implemented for molecular states and lifetimes in LiDB [5] with values determined at vibronic and vibrational-state resolution from rotationally-resolved data. However, a caveat is that the atomic states of the noble gas neutral species Ne, Ar, Kr, and Xe in the NIST ASD are labelled using Racah spectroscopic notation where the atomic term symbols explicitly depend on J. The decision was therefore made to produce J-resolved lifetimes and states for these four species as their states are commonly identified using Racah notation, for example, in the QDB database of plasma chemistries and reactions [10] which uses LiDB data.

Atomic datasets composed of energy levels (in cm^{-1}), atomic term symbols, electronic configurations, J quantum numbers, transitions between states and the respective Einstein A coefficients (in s^{-1}) were extracted from the NIST ASD. Not all atomic states in NIST ASD are assigned and those without labelling were discarded. Similarly, transitions without Einstein A coefficients were ignored. Atomic data in the NIST ASD corresponds to the natural abundance of isotopes and the same therefore applies to atomic data in LiDB. States and transitions were considered up to $n_{\text{outer}} + 2$ for each atom, where n_{outer} is the principal quantum number of the outermost electron. For example, in hydrogen we consider states and transitions up to $n = 3$.

Briefly summarizing the algorithm and procedure, lumped atomic states were formed for every unique combination of atomic term symbol and electronic configuration, corresponding to a grouped set of J energy levels. The energy of the lumped state was assigned as the lowest energy J value within the grouped set. Transitions between the lumped states were evaluated to establish partial and total lifetimes, discarding any transitions between different J energy levels within a lumped state. LiDB only provides five partial lifetimes per lumped state, which reduces the size of the datasets but still captures the main radiative emission pathways. Therefore, as a final step the partial lifetimes from a lumped state were renormalized to be consistent with the value for the total lifetime of the lumped state.

To illustrate the procedure, it is informative to consider an atom with $K = 1 \ldots N$ lumped states. In each lumped state, defined by an atomic term and electronic configuration, are multiple J energy levels. An arbitrary upper lumped state U_K contains a set of J-resolved levels (n_u in total) labelled $\{u_1^K, u_2^K, \ldots, u_{n_u}^K\}$. Similarly, an arbitrary lower lumped state L_K contains its own set of J-resolved levels (n_l in total) labelled $\{l_1^K, l_2^K, \ldots, l_{n_l}^K\}$.

All transitions between the upper lumped state set of J-levels and the lower lumped state set of J-levels were processed with their Einstein A coefficients summed to determine the individual contributions to the partial lifetime. Transitions within a lumped state were discarded. Dropping the superscript K on the upper and lower set of J-levels, the contributions were defined as,

$$\tau_{u_1,l} = \frac{1}{\sum_{k=1}^{n_l} A_{u_1,l_k}}, \tag{2}$$

and

$$\tau_{u_2,l} = \frac{1}{\sum_{k=1}^{n_l} A_{u_2,l_k}}, \tag{3}$$

and so on, up to $\tau_{u_{n_u},l}$. Here, A_{u_1,l_1} is the Einstein A coefficient of the transition between the energy levels $u_1 \rightarrow l_1$.

The partial lifetime $\tau_{U,L}$ (in seconds) between an upper and lower lumped state was obtained from the weighted sum of the individual contributions,

$$\tau_{U,L} = \frac{1}{W} \sum_{k=1}^{n_u} \tau_{u_k,l} \times g_{\text{tot}}^{u_k}, \tag{4}$$

where

$$W = \sum_{k=1}^{n_u} g_{\text{tot}}^{u_k}, \tag{5}$$

and the total statistical degeneracy factor $g_{\text{tot}}^{u_k} = (2J + 1)$ for the energy level u_k. The lumping procedure accounts for the different statistical weights but does not account for the eventual different

populations of the excited states due to non-thermal structure effects, for example, differences caused by the excitation of electrons described by the electron energy distribution function (EEDF) for the specific plasma.

Partial lifetimes were computed between all the connected upper and lower lumped states in an atom. The energy difference between the lower and upper lumped state $\Delta E = E_L - E_U$ was always negative, i.e., corresponding to radiative decay. Summing the partial lifetimes from an upper (decaying) lumped state to the connected lower lumped states yields the total lifetime.

For example, considering an arbitrarily chosen upper lumped state U_3 connected to the lower lumped states L_2, L_1, and L_0, summing the partial lifetimes,

$$C_3 = \frac{1}{\tau_{U_3,L_2}} + \frac{1}{\tau_{U_3,L_1}} + \frac{1}{\tau_{U_3,L_0}}, \tag{6}$$

leads to the total lifetime τ_{U_3} of the upper lumped state U_3 as,

$$\tau_{U_3} = \frac{1}{C_3}. \tag{7}$$

More generally, the relationship is expressed as

$$C_K = \sum_{j=0}^{K-1} \frac{1}{\tau_{U_K,L_j}}, \tag{8}$$

and

$$\tau_{U_K} = \frac{1}{C_K}, \tag{9}$$

for $K = 1, \ldots, N$ lumped states in an atom.

The number of partial lifetimes between atomic states substantially increases for more complex systems such as iron. Plasma modelling is primarily interested in the dominant decay pathways and for this reason LiDB provides no more than five values per lumped state. This number was chosen to capture the primary decay paths while reducing the size of the datasets. Since the total lifetimes are constructed from a summation involving all of the partial lifetimes, see Eqs. (8) and (9), the five shortest partial lifetimes must be renormalized such that their summation still equals the total lifetime.

Renormalization was carried out using a renormalization factor R_K determined for each lumped state from $K = 1, \ldots, N$. This was defined as the ratio between the total lifetime τ_{U_K} and a "reduced" total lifetime $\tau^*_{U_K}$ calculated from summing the five shortest partial lifetimes from the same upper lumped state, that is

$$R_K = \frac{\tau_{U_K}}{\tau^*_{U_K}}. \tag{10}$$

The renormalization factor was applied to the partial lifetimes,

$$\tau^*_{U_K,L} = R_K \times \tau_{U_K,L}, \tag{11}$$

to produce renormalized partial lifetimes which are provided in LiDB. No renormalization was applied to the total lifetimes.

The J-resolved total and partial lifetimes of the noble gas neutral species Ne, Ar, Kr, and Xe were calculated in a straightforward manner without any lumping procedure. The total lifetimes of the atomic states were determined using Eq. (1). Partial lifetimes were simply $1/A_{if}$, where A_{if} is the Einstein A coefficient of the transition connecting the upper and lower states. Partial lifetimes were renormalized as described above.

All atomic ground states possess an infinite lifetime in LiDB. A small number of higher energy states with no transitions linking them to states lower in energy, often metastable states which do not decay radiatively, were also assigned infinite lifetimes. It is worth mentioning that atomic transition data in the NIST ASD, although relatively comprehensive for the species considered, are incomplete. This will affect the values of the lifetimes and unfortunately there is no way of knowing the completeness of an atomic line list on NIST. Users should therefore exercise caution for atomic lifetime values that seem irregular. Molecular data in LiDB is not affected by this issue as lifetimes were generated from complete molecular line lists from the ExoMol database.

Table 1
List of neutral atoms currently in LiDB. N_{states} is the number of atomic states and hence radiative lifetimes, N_{trans} is the number of provided partial lifetimes between the states, and E_{thresh} is the upper energy threshold of the dataset (in eV).

Atom	N_{states}	N_{trans}	E_{thresh} (eV)
Al	14	28	5.476
Ar	76	231	15.351
As	6	5	7.540
B	19	35	12.011
Be	19	32	8.528
Br	21	27	11.053
C	42	160	13.117
Ca	30	32	6.016
Cl	22	32	11.993
Cr	116	180	8.051
Cu	14	19	7.737
F	18	41	17.058
Fe	150	559	7.509
Ga	6	5	5.402
Ge	8	11	6.377
H	6	8	12.087
He	11	25	23.086
K	13	25	3.962
Kr	53	154	13.492
Li	9	17	4.541
Mg	27	70	10.354
Mn	94	163	8.520
N	45	160	15.027
Na	18	37	36.252
Ne	53	207	20.805
Ni	66	191	7.151
O	45	94	17.774
P	21	27	9.884
S	36	63	10.097
Sc	41	65	5.856
Si	47	148	7.667
Ti	84	148	5.820
V	121	298	6.196
Xe	47	100	11.877
Zn	11	10	16.196

The neutral and singly-charged atomic species that have been processed for LiDB are listed in Table 1 and Table 2, respectively. Listed for each dataset is the number of atomic states and hence radiative lifetimes, the number of partial lifetimes between the states, and the upper energy threshold (in eV). A total of 35 neutral and 19 singly-charged atomic species are currently available. Note that it is commonplace for neutral and singly-charged species to be described by the notation, e.g. for carbon as C I and C II whereas we have opted for the notation C and C^+ to be consistent with the ExoMol [6–9] and QDB [10] databases.

In Fig. 1, total radiative lifetimes τ (in seconds) of neutral carbon (C), silicon (Si), argon (Ar), and iron (Fe) are plotted against the energy (in eV) of the radiative state. A comparison is shown of lifetimes computed using the LiDB state-lumping procedure, denoted as lumped lifetimes, against the standard J-resolved lifetimes obtained using Eq. (1). The lumped lifetimes closely follow the J-resolved values, demonstrating the validity of our approach. Evidently, state lumping captures the main radiative behaviour of a species but reduces the number of lifetimes. For example, in carbon there are 42 lumped lifetimes compared to 72 J-resolved values. In more complex systems this reduction is larger, for example, in iron there are 150 lumped lifetimes compared to 409 J-resolved values.

3. LiDB database overview

LiDB is freely available and hosted at www.exomol.com/lidb, see Figs. 2 and 3. Users can dynamically view atomic and molecular datasets or request data through an application programming interface (API). On the homepage is the list of species contained in LiDB. For

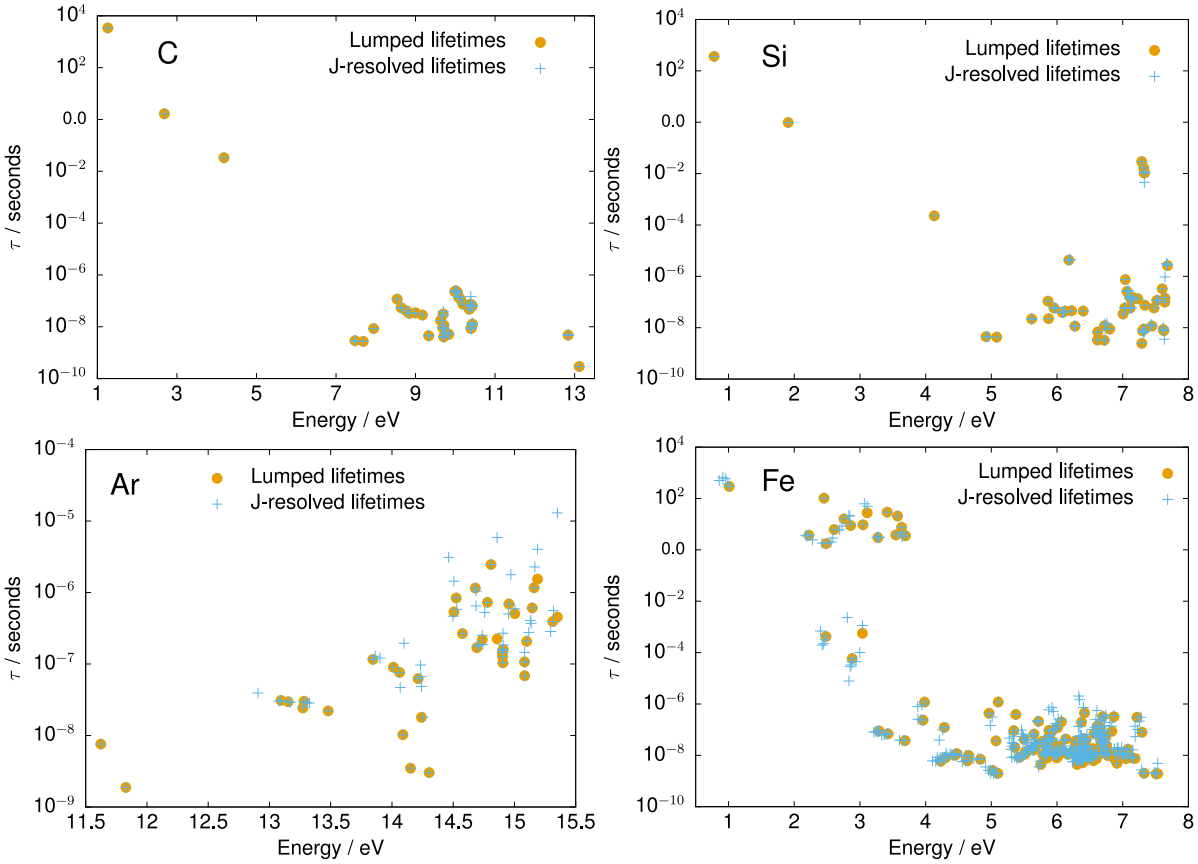

Fig. 1. Radiative lifetimes τ (in seconds) for lumped states of neutral carbon (C), silicon (Si), argon (Ar) and iron (Fe) compared against J-resolved lifetimes. Note that the lifetime of the ground state is infinite and not shown in the figures. For Ar, the metastable states at 11.548 eV and 11.723 eV have infinite lifetimes in LiDB and are not shown in the figure (but are present in the database).

Table 2
List of singly-charged atoms currently in LiDB. N_{states} is the number of atomic states and hence radiative lifetimes, N_{trans} is the number of provided partial lifetimes between the states, and E_{thresh} is the upper energy threshold of the dataset (in eV).

Atom	N_{states}	N_{trans}	E_{thresh} (eV)
Al^+	31	67	18.658
Ar^+	36	93	24.825
B^+	32	101	24.856
Be^+	9	16	14.809
C^+	35	93	27.377
Cl^+	44	49	22.891
F^+	19	14	32.849
He^+	6	5	48.370
Kr^+	11	9	19.575
Li^+	11	25	69.647
Mg^+	11	30	12.856
N^+	47	181	30.367
Na^+	18	63	69.950
Ne^+	35	69	38.023
O^+	46	164	34.217
P^+	20	22	16.336
S^+	55	151	22.090
Si^+	24	56	16.339
Xe^+	16	14	16.936

atoms, clicking on a species will bring up basic information such as the main isotope, i.e., the largest contributor at natural abundance, mass (in Da), the total number of states corresponding to the number of lifetimes, and the total number of transitions corresponding to the number of partial lifetimes.

Atomic data is separated into two categories: states and transitions. The states category lists the atomic states, their energies (in eV), and the total radiative lifetimes (in seconds). Each state is uniquely labelled with an atomic term symbol and electronic configuration, defined and formatted using PyValem [15,16], which is a Python package for specifying atomic and molecular species and states in a standardized way. As discussed above, the spectroscopic notation and convention of each state and species was directly adopted from the respective entries in the NIST ASD. The transitions category provides partial lifetimes for up to five emission pathways per state. Users can view the initial and final state, the change in energy ΔE (in eV) which is always negative as the final state is lower in energy than the initial state, and the partial lifetime (in seconds). There is also functionality to look at individual states and the specific transitions to and from them.

A detailed description with examples of how to request data through the API is provided on the website. Requests are made using the GET protocol and require certain keywords to retrieve the correct atomic data. Requests must be made using the `molecule` keyword to select a specific dataset, even for requesting atomic data, e.g., `molecule=C` for neutral carbon or `molecule=C+` for singly-charged carbon. Datasets are split into two categories. Setting the keyword `category=states` will request total radiative lifetimes (in seconds) for the atomic states, while `category=transitions` will request partial lifetimes (in seconds) between states. Data can be returned in either JSON (default)

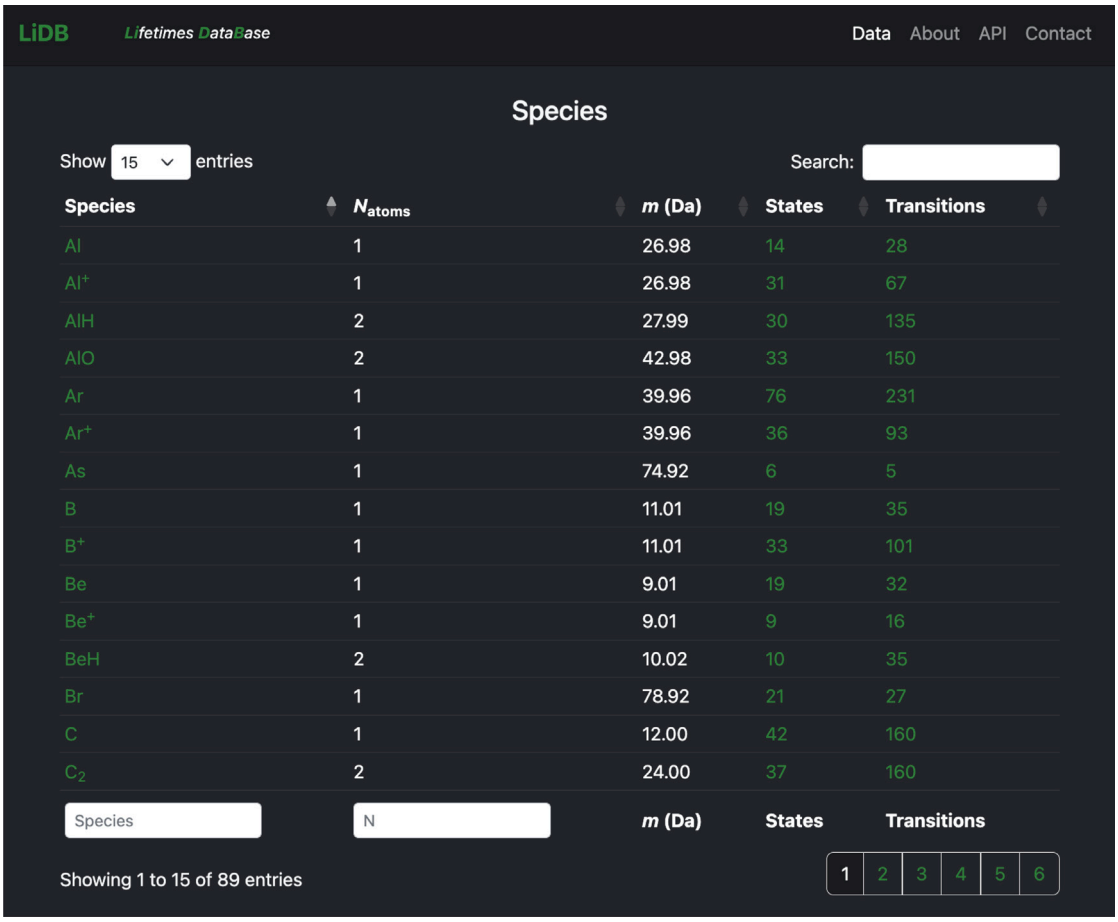

Fig. 2. Screenshot of the LiDB website at www.exomol.com/lidb. Users can view atomic and molecular datasets dynamically or use the API to query the database.

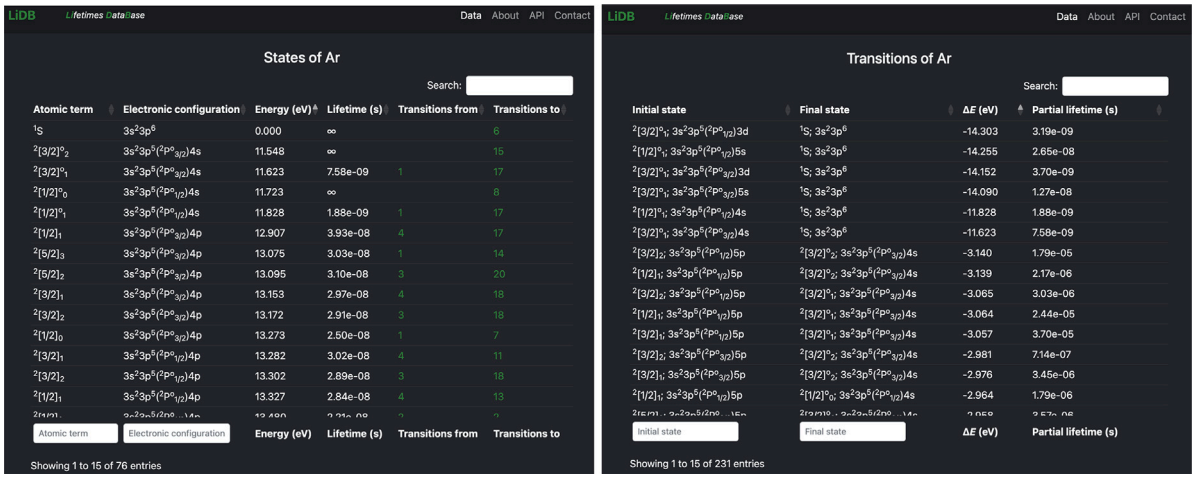

Fig. 3. Screenshot of the LiDB website at www.exomol.com/lidb. The left panel shows atomic states and total radiative lifetimes of neutral argon (Ar). The right panel shows transitions between the states and partial lifetimes of neutral argon (Ar).

or CSV format. For example, requesting radiative lifetimes of neutral hydrogen in CSV format can be done using the following command:

```
https://www.exomol.com/lidb/api/
?molecule=H&category=states&format=csv
```

and this will return a comma-separated values file with three columns listing the atomic state (PyValem notation), lifetime (in s) and energy (in eV).

4. Conclusions

Atomic radiative lifetimes for neutral and singly-charged species have been added to the LiDB database, enhancing the existing offering of molecular radiative data. Atomic datasets were generated from energy levels, transitions and Einstein A coefficients extracted from the NIST ASD. The procedure involved forming lumped atomic states and averaging over the effects of the total angular momentum quantum number J. Total radiative lifetimes and partial lifetimes of

up to five of the most dominant decay channels from each state were produced. A total of 35 neutral and 19 singly-charged species have been processed and all datasets are freely available at www.exomol.com/lidb, where users can dynamically view data on the website or perform data requests through an API. LiDB will help capture radiative effects in the modelling of low-temperature plasmas and is a valuable addition to existing atomic databases (see Ref. [17] and the associated articles in the Atoms journal special issue on the Development and Perspectives of Atomic and Molecular Databases). Users are encouraged to contact us with requests for atomic and molecular data that they would like to be added to LiDB. The ExoMol database [6–9] is also currently adding detailed atomic spectroscopic data and this will be another complementary resource for studies of radiative states in plasmas.

CRediT authorship contribution statement

Alec Owens: Writing – original draft, Software, Methodology, Investigation, Data curation, Conceptualization. **Tingting Chen:** Software, Formal analysis. **Christian Hill:** Writing – review & editing, Software, Data curation. **Sebastian Mohr:** Validation, Conceptualization. **Jonathan Tennyson:** Writing – review & editing, Supervision, Funding acquisition, Conceptualization.

Declaration of competing interest

JT and SB are both Directors of Quantemol Ltd.; Quantemol are interested in utilizing the results of this study.

The other authors declare no conflict of interest.

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Data availability

The LiDB atomic and molecular data discussed in this article are all available at www.exomol.com/lidb/molecule/list/all. Atomic data is based on data from the NIST Atomic Spectra Database at www.nist.gov/pml/atomic-spectra-database while molecular data is based on data from the ExoMol database at www.exomol.com.

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