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EXOATOM: a database of atomic spectra in ExoMol format

Qing-He Ni[1] Rujia Wang,[1] Tianyang Xie,[1] Jingxin Zhang[1,2] Christian Hill[3] Sergei N. Yurchenko[1] and Jonathan Tennyson[1★]

[1]*Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, UK*
[2]*State Key Laboratory of High Temperature Gas Dynamics, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100190, China*
[3]*International Atomic Energy Agency, Vienna A-1400, Austria*

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ABSTRACT

We present the EXOATOM database, an extension of the ExoMol database to provide atomic line lists in the ExoMol format. EXOATOM is designed for detailed astrophysical, planetary, and laboratory applications. EXOATOM currently includes atomic data for 80 neutral atoms and 74 singly charged ions. These data are extracted from both the NIST and Kurucz databases, with 79/71 atoms/ions sourced from NIST and 38/37 atoms/ions sourced from Kurucz. EXOATOM uses the file types `.all`, `.def`, `.states`, `.trans`, and `.pf` as fundamental components for structuring atomic data in a consistent hierarchy. The `.states` file contains quantum numbers, uncertainties, lifetimes, etc. The `.trans` file specifies Einstein *A* coefficients and their associated wavenumbers. The `.pf` file provides partition functions over a wide grid of temperatures. Post-processing of the EXOATOM data is provided by the program PYEXOCROSS. Future development of EXOATOM will include additional ionization stages.

Key words: Data Methods – EXOMOL – Atom – Database.

1 INTRODUCTION

The ExoMol database was established in 2011 to provide molecular line lists for exoplanet and other atmospheres (J. Tennyson & S. N. Yurchenko 2012). Given their importance the ExoMol database included contributions due to atomic sodium (N. F. Allard et al. 2019) and potassium (N. F. Allard, F. Spiegelman & J. F. Kielkopf 2016) in its opacity tables (K. L. Chubb et al. 2021). However, spectra of many neutral and singly ionized atoms are a regular feature of high resolution studies of exoplanetary atmospheres (L. Fossati et al. 2010; J. L. Linsky et al. 2010; J. J. Spake et al. 2018; H. J. Hoeijmakers et al. 2019, 2020, 2024; Z. Jiang et al. 2023; S. Pelletier et al. 2023; M. C. D'Arpa et al. 2024; A. Simonnin et al. 2024). For example, B. Prinoth et al. (2025) considered the spectra of 89 neutral or singly ionized atoms in their analysis of the ultrahot Jupiter exoplanet WASP-121 b and assigned features due to 17 of them in a study in which they also searched for the spectral signature of TiO. The increasing need for atomic spectra to be used alongside molecular spectra in exoplanets, and indeed other astronomical objects, has led to users requesting us to expand the ExoMol database to explicitly include atomic line spectra. As this expansion more than doubles the number of species included in the ExoMol database and because there are some subtle differences in the data presented for atoms and molecules, we have chosen to create a new database section of the ExoMol database presenting atomic data called EXOATOM, while retaining the original ExoMol branding for the molecular line lists (J. Tennyson et al. 2024). As detailed below, EXOATOM uses the same data structure as the molecular section of the ExoMol database and retains many of its characteristics.

There are a number of existing databases which provide atomic spectroscopic data which are used in astronomical studies. These include the Atomic Spectra Database of the National Institute of Standards and Technology (Y. Ralchenko & A. Kramida 2020) (henceforth simply NIST), the line list compilations due to R. L. Kurucz (2011, 2018), VALD3 (the third edition of the Vienna Atomic Line Database) (T. Ryabchikova et al. 2015), CHIANTI – An Atomic Database for Emission Lines (G. Del Zanna et al. 2021), and the Opacity Project (M. J. Seaton 2005) including the more focused spin-off Iron Project (C. Mendoza 2000). EXOATOM contains data extracted from the NIST and Kurucz databases. These two databases provided complementary information with NIST providing a more limited, high accuracy set of spectroscopic parameters largely based on precision laboratory measurements while the Kurucz line lists aim at completeness with many of the results coming from quantum mechanical calculations.

Here we present the EXOATOM database, which aims to expand the ExoMol database by providing atomic line lists derived from both the NIST and Kurucz databases in the ExoMol format.

2 DATA COVERAGE

Below is a detailed description of the EXOATOM data coverage. Table 1 summarizes the final contents of the EXOATOM database. Tables 2 and 3 list the total number of energy states and transition lines for each atom and ion, respectively, in the NIST data set. Tables 4 and 5 provide the corresponding counts of states and lines for each atom and ion in the Kurucz database.

★ E-mail: j.tennyson@ucl.ac.uk

Table 1. Data coverage of the ExoAtom database.

Category	Atom count	NIST	Kurucz
Neutral atoms	80	79	38
Singly charged ions	74	71	37

3 DATABASE STRUCTURE

The Django web framework is used for the database implementation of ExoAtom, written in the Python programming language (A. Holovaty et al. 2003). The ExoAtom data structure is an extension of the original ExoMol data structure (J. Tennyson, C. Hill & S. N. Yurchenko 2013; J. Tennyson et al. 2024), see J. Tennyson et al. (2023). This data structure is designed to offer a full description of the metadata for each file; it can be routinely used for both downloading and updating data through an application program interface (API), see J. Tennyson et al. (2024).

While the majority of the molecular data in ExoMol were generated in-house, atomic data are not natively produced by the ExoMol team. Therefore, the contents of ExoAtom have been taken from existing atomic spectroscopic databases: NIST and Kurucz. Then, to ensure consistency with ExoMol formatting, a systematic approach is taken to extract, process, and convert data from these sources. After having been scraped from the original databases, the atomic data for each element are then converted to the three primary, ExoMol-formatted files: the `.states` file, the transitions `.trans` file, and the partition function `.pf` file.

The following section provides a detailed review of the ExoMol format and precisely which data were scraped from the NIST and Kurucz databases to supply the atomic data for ExoAtom.

As specified in Table 6, the major difference between the two data sets is that NIST aims for accuracy while Kurucz aims for completeness. Which of these properties is more important will depend on individual use cases so, in contrast to the molecular line lists provided by ExoMol, we do not recommend a data set for each atom or ion. Instead this choice needs to be made by the user based on their particular data requirements.

3.1 ExoMol format

The ExoMol database consists of 15 types of files, as summarized in Table 7.

The ExoAtom database selects the `.all`, `.def`, `.states`, `.trans`, and `.pf` files from ExoMol as fundamental components for structuring atomic data (see Table 8). The `.states` file contains energy levels along with their quantum numbers, uncertainties, lifetimes, term, etc. Optionally the `.states` file can provide Landé g-factors which can be used to give the splitting of levels in weak magnetic fields. For each transition, the `.trans` file provides identifiers to the two states involved, the associated Einstein A coefficient and corresponding wavenumbers. The `.pf` file provides partition functions over a range of temperatures.

3.2 NIST databases

The NIST Atomic Spectra Database was accessed via the NIST Atomic Spectra Database website (A. Kramida et al. 2015; Y. Ralchenko & A. Kramida 2020; Y. Ralchenko 2024b), and the data were scraped by R. Wang (2024) in June 2024. This database is essentially a compilation of available, high accuracy experimental measurements which, up to and including 2024, was updated annually.

The NIST database consists of four primary sections: Lines, Levels, Ground States & Ionization Energies, and Laser-Induced Breakdown Spectroscopy (LIBS). Data are extracted from the NIST Atomic Spectra Database Lines section and the Levels section for both neutral and singly charged atoms. The `.states` files are constructed from the energy levels data, while the `.trans` files incorporate both levels and spectral lines data. The `.pf` files are derived from the levels data. The NIST database includes lifetime data for some atomic states but lacks Landé g-factors. Landé g-factors are optional in the ExoMol data structure and are not provided for the NIST data sets. These quantities are important because they enable predictions of Zeeman splitting of rovibronic lines in the presence of magnetic fields, providing a remote-sensing probe of astrophysical environments.

Uncertainties (Unc) of the energy levels of the NIST data were determined as follows. Generally, the uncertainty would be taken directly from NIST. If the NIST uncertainty value ‘Unc’ was absent (‘_’ or blank), it was estimated based on the number of decimal places (N) in the Level data set, using the formula $\mathrm{Unc} = 2 \times 10^{-N}\ \mathrm{cm}^{-1}$. For example, if Level (cm^{-1}) = 12345.24, then the corresponding Unc is 0.02. If Level (cm^{-1}) contains a decimal point but no decimal places (e.g. ‘74728.’), Unc is set to 2.

Due to the absence of valid Einstein A coefficients for certain radioactive elements, the `.trans` files scraped from NIST are absent for elements such as Polonium (Po), Astatine (At), Radon (Rn), and Francium (Fr). These elements exhibit short half-lives, making experimental measurements particularly challenging and limit the likelihood of their astronomical detection. However, `.states` and `.pf` files are available for these atoms.

In some cases, the lines containing valid A_{ki} (s^{-1}) lack valid E_i, E_k, configuration labels (conf_i, conf_k), or terms in the corresponding rows, thus making their correlation to the states impossible. In these cases, the Einstein A coefficients were excluded.

The NIST database provides partition functions within individual HTML files, but each file only allows retrieval for a single temperature. Consequently, obtaining partition functions across a temperature range from 1 K to 6000 K requires extracting data from 6000 separate documents. We have therefore computed these partition function by direct summation, see discussion below.

3.3 Kurucz database

The Kurucz Atomic Line Lists were accessed via the Kurucz Atomic Database website (R. L. Kurucz 2024, 2011) and the data were scraped by T. Xie (2024) in June 2024. The Kurucz database appears to have been last updated in 2017.

In the Kurucz database each neutral atom and singly charged ion are designated by a four-digit identifier (`xxyy`), where `xx` corresponds to the atomic number and `yy` indicates whether the species is neutral (`yy` = `00`) or singly charged (`yy` = `01`). The Kurucz line lists are calculated although some energy data has been replaced by values taken (at an unspecified date) from NIST; these updates are marked in the database. The Kurucz database does not provide the A coefficients directly but instead includes $\log_{10} A$ values in the `.agafgf` files. For certain atoms (S I, Ni II, Nb II, Mo II), the Kurucz atomic `lines` files are not available within the specified path. The Kurucz database provides Landé g-factors (stored in files gfxxyy.gam) and lifetimes (stored in lifexxyy.dat or gfxxyy.life files). However, these lifetime values are not always complete or consistently available; missing values were therefore recomputed using the program PyExoCross (J. Zhang, J. Tennyson & S. N. Yurchenko 2024).

Table 2. Summary of neutral atoms (including isotopes) with `.trans` and `.states` files from NIST including numbers of states ($N_{\rm state}$), number of transitions ($N_{\rm trans}$) and source references.

Element	$N_{\rm state}$	$N_{\rm trans}$	References
^{1}H I	105	441	O. Jitrik & C. F. Bunge (2005), A. E. Kramida (2010)
^{2}H I	77	161	W. L. Wiese & J. R. Fuhr (2009), A. E. Kramida (2010)
^{3}H I	9	11	W. L. Wiese & J. R. Fuhr (2009), A. E. Kramida (2010)
^{4}He I	842	2289	W. L. Wiese & J. R. Fuhr (2009), D. Z. Kandula et al. (2010)
Li I	181	257	R. L. Kelly (1987), W. L. Wiese & J. R. Fuhr (2009)
Be I	212	394	J. R. Fuhr & W. L. Wiese (2010), E. C. Cook, A. D. Vira & W. D. Williams (2020)
B I	118	242	A. E. Kramida & A. N. Ryabtsev (2007), J. R. Fuhr & W. L. Wiese (2010)
C I	433	1616	K. Haris & A. Kramida (2017), W. L. Wiese & J. R. Fuhr (2007)
N I	366	1287	K. Pachucki (2024), W. L. Wiese & J. R. Fuhr (2007)
O I	580	854	W. L. Wiese, J. R. Fuhr & T. M. Deters (1996), G. Demirdak, E. Sahin & M. Ertürk (2023)
F I	302	120	J. Musielok et al. (1999), K. Pachucki (2024)
Ne I	374	533	M. J. Seaton (1998), E. B. Saloman & C. J. Sansonetti (2005)
Na I	423	523	D. E. Kelleher & L. I. Podobedova (2008a), J. E. Sansonetti (2008a)
Mg I	303	1090	W. C. Martin & R. Zalubas (1980), D. E. Kelleher & L. I. Podobedova (2008a)
Al I	185	293	W. C. Martin & R. Zalubas (1979), D. E. Kelleher & L. I. Podobedova (2008a)
Si I	406	603	W. C. Martin & R. Zalubas (1983), D. E. Kelleher & L. I. Podobedova (2008c)
P I	284	132	W. C. Martin, R. Zalubas & A. Musgrove (1985), W. L. Wiese, M. W. Smith & B. M. Miles (1969)
S I	377	913	W. C. Martin, R. Zalubas & A. Musgrove (1990), L. I. Podobedova, D. E. Kelleher & W. L. Wiese (2009)
Cl I	366	99	L. J. Radziemski & V. Kaufman (1969), W. L. Wiese et al. (1969)
Ar I	503	428	J. R. Fuhr & W. L. Wiese (1996),L. Minnhagen (1973)
K I	296	211	J. E. Sansonetti (2008b), W. L. Wiese et al. (1969)
Ca I	780	136	W. L. Wiese et al. (1969), J. Sugar & C. Corliss (1985)
Sc I	355	257	J. Sugar & C. Corliss (1985), G. A. Martin, J. R. Fuhr & W. L. Wiese (1988)
Ti I	558	496	E. B. Saloman (2012a), G. A. Martin et al. (1988)
V I	548	1162	E. B. Saloman & A. Kramida (2017b)
Cr I	618	522	G. A. Martin et al. (1988), E. B. Saloman (2012b)
Mn I	536	489	J. Sugar & C. Corliss (1985), G. A. Martin et al. (1988)
Fe I	837	2542	G. Nave et al. (1994), J. R. Fuhr & W. L. Wiese (2006)
Co I	277	336	J. Sugar & C. Corliss (1985), J. R. Fuhr, G. A. Martin & W. L. Wiese (1988)
Ni I	287	522	J. R. Fuhr et al. (1988), U. Litzén, J. W. Brault & A. P. Thorne (1993)
Cu I	360	37	J. Sugar & A. Musgrove (1990), D. C. Morton (2003)
Zn I	374	16	J. Sugar & A. Musgrove (1995), D. C. Morton (2003)
Ga I	257	23	D. C. Morton (2003), T. Shirai et al. (2007)
Ge I	618	26	W. L. Wiese & G. A. Martin (1980), J. Sugar & A. Musgrove (1993)
As I	84	14	R. L. Kelly (1987), W. L. Wiese & G. A. Martin (1989)
Br I	264	54	C. J. Humphreys, E. Paul & L. Minnhagen (1971), T. Wujec et al. (1999)
Kr I	527	184	D. C. Morton (2000), E. B. Saloman (2007)
Rb I	239	40	J. E. Sansonetti (2006)
Sr I	377	86	J. E. Sansonetti & G. Nave (2010)
Y I	176	189	X. Shang et al. (2015), G. Gil & A. Gonzalez (2017)
Mo I	281	498	J. Sugar & A. Musgrove (1988), W. Whaling & J. W. Brault (1988)
Tc I	274	13	P. Palmeri & J.-F. Wyart (1999), J. E. Sansonetti & W. C. Martin (2005)
Ru I	228	11	C. L. Callender, P. A. Hackett & D. M. Rayner (1988), J. E. Sansonetti & W. C. Martin (2005)
Rh I	75	111	C. L. Callender et al. (1988), J. R. Fuhr & W. L. Wiese (2005)
Pd I	143	8	R. Engleman et al. (1998), J. E. Sansonetti & W. C. Martin (2005)
Ag I	104	7	W. L. Wiese & G. A. Martin (1980), T. Badr et al. (2006)
Cd I	126	18	W. L. Wiese & G. A. Martin (1980), E. Vidolova-Angelova et al. (1996)
In I	111	27	D. C. Morton (2000), H. Karlsson & U. Litzén (2001)
Sn I	218	55	C. M. Brown, S. G. Tilford & M. L. Ginter (1977), W. L. Wiese & G. A. Martin (1980)
Sb I	145	10	F. Hassini et al. (1988), J. E. Sansonetti & W. C. Martin (2005)
Te I	119	6	Y. Makdisi & K. S. Bhatia (1982), D. C. Morton (2000)
I I	220	5	D. Cerny et al. (1991), J. E. Sansonetti & W. C. Martin (2005)
Xe I	443	187	D. C. Morton (2000), E. B. Saloman (2004)
Cs I	178	42	J. E. Sansonetti (2009)
Ba I	355	109	W. L. Wiese & G. A. Martin (1980),J. J. Curry (2004)
La I	206	279	E. A. Den Hartog, A. J. Palmer & J. E. Lawler (2015), W. C. Martin, W. L. Wiese & A. Kramida (2023)
Ce I	354	54	J. E. Lawler et al. (2010), W. C. Martin et al. (2023)
Nd I	229	4	J. E. Sansonetti & W. C. Martin (2005), W. C. Martin et al. (2023)
Sm I	220	7	J. E. Sansonetti & W. C. Martin (2005), W. C. Martin et al. (2023)
Eu I	316	142	D. C. Morton (2000), W. C. Martin et al. (2023)
Gd I	465	16	W. C. Martin et al. (2023), J. E. Sansonetti & W. C. Martin (2005)
Dy I	302	40	W. L. Wiese & G. A. Martin (1980), J. E. Sansonetti & W. C. Martin (2005)

Table 2 – *continued*

Element	$N_{\rm state}$	$N_{\rm trans}$	References
Ho I	201	12	J. E. Sansonetti & W. C. Martin (2005), W. C. Martin et al. (2023)
Er I	313	10	J. E. Sansonetti & W. C. Martin (2005), W. C. Martin et al. (2023)
Tm I	477	349	M. E. Wickliffe & J. E. Lawler (1997a), W. C. Martin et al. (2023)
Yb I	182	5	J. E. Sansonetti & W. C. Martin (2005), W. C. Martin et al. (2023)
Lu I	198	44	J. Vergès & J.-F. Wyart (1978), J. A. Fedchak et al. (2000)
Hf I	278	187	D. W. Duquette, E. A. Den Hartog & J. E. Lawler (1986), J. E. Lawler, J. R. Schmidt & Hartog E. A. DenHartog (2022)
Ta I	122	135	V. Fivet et al. (2006a), W. C. Martin et al. (2023)
W I	144	121	A. E. Kramida & T. Shirai (2006)
Ir I	53	37	H. L. Xu et al. (2007), W. C. Martin et al. (2023)
Pt I	184	166	J. Blaise et al. (1992), E. A. Den Hartog et al. (2005)
Au I	61	20	J. E. Sansonetti & W. C. Martin (2005), V. Fivet et al. (2006b)
Hg I	294	53	J. R. Fuhr & W. L. Wiese (2005), E. B. Saloman (2006)
Tl I	66	9	W. L. Wiese & G. A. Martin (1980), W. C. Martin et al. (2023)
Pb I	134	28	D. R. Wood & K. L. Andrew (1968), D. C. Morton (2000)
Bi I	71	39	G. M. Wahlgren et al. (2001), S. Werbowy & J. Kwela (2009)
Fr I	122	149	J. R. Fuhr & W. L. Wiese (2005), J. E. Sansonetti (2007)
Ra I	81	19	W. L. Trimble et al. (2009), U. Dammalapati, K. Jungmann & L. Willmann (2016)
Ac I	52	91	A. Kramida (2022)

Table 3. Summary of singly charged atoms (including isotopes) with `.trans` and `.states` files from NIST including $N_{\rm state}$, $N_{\rm trans}$ and source references.

Element	$N_{\rm state}$	$N_{\rm trans}$	References
^{3}He II	148	140	W. L. Wiese & J. R. Fuhr (2009), V. A. Yerokhin & V. M. Shabaev (2015)
^{4}He II	148	140	O. Jitrik & C. F. Bunge (2005), V. A. Yerokhin & V. M. Shabaev (2015)
Li II	178	564	G. W. Drake (1988), W. L. Wiese & J. R. Fuhr (2009)
Be II	249	149	J. R. Fuhr & W. L. Wiese (2010), A. E. Kramida (2005)
B II	156	435	A. N. Ryabtsev et al. (2005), J. R. Fuhr & W. L. Wiese (2010)
C II	414	1433	A. Kramida & K. Haris (2022)
N II	178	786	J. Musielok et al. (1996), Y. Sun et al. (2021)
O II	275	876	W. L. Wiese et al. (1996), G. Gil & A. Gonzalez (2017)
F II	290	67	W. L. Wiese, M. W. Smith & B. M. Glennon (1966), R. L. Kelly (1987)
Ne II	380	233	W. L. Wiese et al. (1966), A. Kramida & G. Nave (2008)
Na II	162	176	D. E. Kelleher & L. I. Podobedova (2008a), J. E. Sansonetti (2008a))
Mg II	137	482	W. C. Martin & R. Zalubas (1980), D. E. Kelleher & L. I. Podobedova (2008a)
Al II	217	986	W. C. Martin & R. Zalubas (1979), D. E. Kelleher & L. I. Podobedova (2008b)
Si II	148	474	W. C. Martin & R. Zalubas (1983), D. E. Kelleher & L. I. Podobedova (2008c
P II	160	73	W. L. Wiese et al. (1969), W. C. Martin et al. (1985)
S II	232	753	W. C. Martin et al. (1990), L. I. Podobedova et al. (2009)
Cl II	274	221	W. L. Wiese et al. (1969), L. J. Radziemski & V. Kaufman (1974)
Ar II	418	307	W. L. Wiese et al. (1969), E. B. Saloman (2010)
K II	96	252	J. E. Sansonetti (2008b)
Ca II	71	99	W. L. Wiese et al. (1969), J. Sugar & C. Corliss (1985)
Sc II	168	139	J. Sugar & C. Corliss (1985), G. A. Martin et al. (1988)
Ti II	252	470	G. A. Martin et al. (1988), E. B. Saloman (2012a)
V II	407	1884	E. B. Saloman & A. Kramida (2017a)
Cr II	913	92	J. Sugar & C. Corliss (1985), D. C. Morton (2003)
Mn II	514	840	A. Kramida & J. E. Sansonetti (2013)
Fe II	1027	7293	J. R. Fuhr & W. L. Wiese (2006), G. Nave & S. Johansson (2012)
Co II	478	2746	J. Sugar & C. Corliss (1985), A. J. J. Raassen, J. C. Pickering & P. H. M. Uylings (1998)
Ni II	713	208	J. Sugar & C. Corliss (1985), J. R. Fuhr et al. (1988)
Cu II	467	553	A. Kramida, G. Nave & J. Reader (2017)
Zn II	93	22	J. Sugar & A. Musgrove (1995), D. C. Morton (2003)
Ga II	95	10	T. Shirai et al. (2007)
Ge II	127	20	W. L. Wiese & G. A. Martin (1980), J. Sugar & A. Musgrove (1993)
Kr II	162	20	J. R. Fuhr & W. L. Wiese (2005), E. B. Saloman (2007)
Rb II	165	49	J. E. Sansonetti (2006)
Sr II	70	33	J. E. Sansonetti (2012)
Y II	235	66	A. E. Nilsson, S. Johansson & R. L. Kurucz (1991), P. Hannaford et al. (1982)
Tc II	33	6	J. E. Sansonetti & W. C. Martin (2005), G. Gil & A. Gonzalez (2017)
Ru II	225	8	H. Karlsson, A. Joueizadeh & S. Johansson (2002), J. E. Sansonetti & W. C. Martin (2005)

Table 3 – *continued*

Element	N_{state}	N_{trans}	References
Pd II	185	10	H. Lundberg et al. (2001), J. E. Sansonetti & W. C. Martin (2005)
Ag II	99	236	A. Kramida (2013b)
Cd II	95	87	H. L. Xu et al. (2004), G. Gil & A. Gonzalez (2017)
In II	194	528	A. Kramida (2013a)
Sn II	76	134	K. Haris, A. Kramida & A. Tauheed (2014)
Sb II	109	2	J. E. Sansonetti & W. C. Martin (2005), G. Gil & A. Gonzalez (2017)
Xe II	161	22	E. B. Saloman (2004), J. R. Fuhr & W. L. Wiese (2005)
Cs II	315	2	J. E. Sansonetti (2009)
Ba II	161	83	W. L. Wiese & G. A. Martin (1980), J. J. Curry (2004)
La II	109	84	J. E. Lawler, G. Bonvallet & C. Sneden (2001), F. Güzelçimen et al. (2018)
Ce II	480	283	J. E. Lawler et al. (2009), M. S. Safronova, U. I. Safronova & C. W. Clark (2015)
Pr II	111	101	R. Li et al. (2007), L. Radžiūtė et al. (2020)
Nd II	325	99	E. A. Den Hartog et al. (2003), L. Radžiūtė et al. (2020)
Sm II	127	7	J. E. Sansonetti & W. C. Martin (2005), L. Radžiūtė et al. (2020)
Eu II	57	13	J. E. Sansonetti & W. C. Martin (2005), L. Radžiūtė et al. (2020)
Tb II	62	8	J. E. Sansonetti & W. C. Martin (2005)
Dy II	300	17	J. E. Sansonetti & W. C. Martin (2005)
Ho II	31	4	J. E. Sansonetti & W. C. Martin (2005), L. Radžiūtė et al. (2021)
Er II	111	7	J. E. Sansonetti & W. C. Martin (2005), L. Radžiūtė et al. (2021)
Tm II	351	13	J. E. Sansonetti & W. C. Martin (2005), L. Radžiūtė et al. (2021)
Yb II	284	10	J. E. Sansonetti & W. C. Martin (2005), L. Radžiūtė et al. (2021)
Lu II	37	9	J. E. Sansonetti & W. C. Martin (2005), E. V. Kahl et al. (2019)
Hf II	106	2	J. E. Sansonetti & W. C. Martin (2005), S. O. Allehabi, V. A. Dzuba & V. V. Flambaum (2022)
W II	58	71	A. E. Kramida & T. Shirai (2006)
Ir II	53	126	T. A. M. van Kleef & B. C. Metsch (1978), H. L. Xu et al. (2007)
Pt II	277	183	J.-F. Wyart, J. Blaise & Y. N. Joshi (1995), P. Quinet et al. (2008)
Hg II	114	446	C. J. Sansonetti & J. Reader (2001), J. E. Sansonetti & W. C. Martin (2005)
Tl II	76	3	J. E. Sansonetti & W. C. Martin (2005)
Pb II	90	3	J. E. Sansonetti & W. C. Martin (2005)
Bi II	77	4	L. Dolk, U. Litzén & G. M. Wahlgren (2002), J. E. Sansonetti & W. C. Martin (2005)
Ra II	36	9	B. K. Sahoo et al. (2009), U. Dammalapati et al. (2016)
Ac II	83	288	A. Kramida (2022)

Table 4. N_{state} and N_{trans} for each Neutral in Kurucz Database (R. L. Kurucz 2014; R. L. Kurucz et al. 2009; F. Castelli & R. L. Kurucz 2010; R. C. Peterson & R. L. Kurucz 2014, 2022; R. L. Kurucz 2002; F. Castelli, R. L. Kurucz & C. R. Cowley 2015)

Element	N_{state}	N_{trans}	References
Li I	123	1424	W. L. Wiese et al. (1966), T. C. Caves (1975), S. Sengupta (1975), A. Lindgard & S. E. Nielsen (1977)
Be I	663	23574	H. Pfennig, R. Steele & E. Trefftz (1965), W. L. Wiese et al. (1966), C. Laughlin & G. A. Victor (1974), C. Laughlin, E. R. Constantinides & G. A. Victor (1978)
B I	1549	22012	W. L. Wiese et al. (1966), I. Martinson, W. Bickel & A. Olme (1970), J. Bromander (1971), R. L. Kurucz & E. Peytremann (1975)
C I	3500	250828	W. L. Wiese et al. (1966), D. Lambert (1968), J. Bromander (1971), D. C. Morton & W. H. Smith (1973), M. H. Miller et al. (1974), R. L. Kurucz & E. Peytremann (1975), A. Goly (1976), M. Cohen & R. P. McEachran (1978), N. H. Brooks, D. Rohrlich & W. H. Smith (1977), J. Bromander, N. Erman & P. Larsson (1978), M. W. Smith & W. L. Wiese (1971), D. Stuck & B. Wende (1974), H. Nussbaumer & C. Rusca (1979), W. L. Wiese et al. (1996)
N I	4479	356876	W. L. Wiese et al. (1966), C. Nicolaides, O. Sinanoglu & P. Westhaus (1971), P. D. Dumont, E. Biemont & N. Grevesse (1974), R. L. Kurucz & E. Peytremann (1975), N. H. Brooks et al. (1977), W. L. Wiese et al. (1996)
O I	3932	109396	R. L. Kurucz & E. Peytremann (1975), W. L. Wiese et al. (1966, 1996), J. Bromander et al. (1978)
F I	1959	131375	R. L. Kurucz & E. Peytremann (1975)
Ne I	777	15361	R. D. Bengston & M. H. Miller (1970), R. L. Kurucz & E. Peytremann (1975), R. A. Lilly (1975), P. Martin & J. Campos (1977), P. Martin & J. Campos (1978), P. Martin & J. Campos (1979)
Na I	3131	51288	W. L. Wiese et al. (1969), R. L. Kurucz & E. Peytremann (1975), A. Lindgard & S. E. Nielsen (1977)
Mg I	588	22612	B. Warner (1968b), A. R. Schaefer (1971), E. M. Anderson, V. A. Zilitis & E. S. Sorokina (1967), W. H. Smith & H. S. Liszt (1971), W. L. Wiese et al. (1969), H. Friedrich & E. Trefftz (1970), C. Froese Fischer (1975a, b), R. L. Kurucz (1975), C. Laughlin & G. A. Victor (1974), R. L. Kurucz & E. Peytremann (1975), R. Lincke & G. Ziegenbein (1971)
Al I	1888	29081	W. L. Wiese et al. (1969), W. H. Smith & H. S. Liszt (1971), R. L. Kurucz (1975), R. L. Kurucz & E. Peytremann (1975), G. G. Lombardi, B. L. Cardon & R. L. Kurucz (1981), R. A. Roig (1975)
Si I	3177	171085	M. H. Miller (1968), E. Schulz-Gulde (1969), N. Grevess & J. P. Swings (1972), T. Garz (1973), R. L. Kurucz (1975), R. L. Kurucz & E. Peytremann (1975)
P I	2387	202300	W. L. Wiese et al. (1969), M. H. Miller, R. A. Roig & R. D. Bengston (1971), G. M. Lawrence (1967), R. L. Kurucz & E. Peytremann (1975), A. E. Livingston et al. (1975)

Table 4 – *continued*

Element	N_{state}	N_{trans}	References
S I	4171	13026	R. L. Kurucz & E. Peytremann (1975), W. L. Wiese et al. (1969), E. W. Foster (1967)
Cl I	1727	255821	R. L. Kurucz & E. Peytremann (1975)
Ar I	801	49824	S. V. Desai & W. H. Corcoran (1968), W. L. Wiese et al. (1969), G. P. Anisimove & R. I. Semenov (1974), R. L. Kurucz & E. Peytremann (1975), R. A. Lilly (1976), J. Woodyard & P. L. Altick (1979)
K I	2865	88919	M. A. Mazing & P. D. Serapinas (1969), W. L. Wiese et al. (1969), R. L. Kurucz & E. Peytremann (1975)
Ca I	1127	46062	G. H. Newsom (1966), B. Warner (1968a), W. L. Wiese et al. (1969), G. H. Newsom (1968), R. L. Kurucz (1988)
Sc I	4307	724611	W. L. Wiese & J. R. Fuhr (1975), W. H. Parkinson, E. Reeves & F. S. Tomkins (1976), R. L. Kurucz (1988), G. A. Martin et al. (1988)
Ti I	13977	5071484	M. Klemt (1973), S. J. Wolnik & R. O. Berthel (1973), J. Lotrian, J. Cariou & A. JohanninGilles (1975), W. L. Wiese & J. R. Fuhr (1975), R. L. Kurucz (1988), G. A. Martin et al. (1988), P. L. Smith & M. Kuhne (1978)
V I	29719	7056409	R. B. King (1947a), R. L. Kurucz (1988), G. A. Martin et al. (1988)
Cr I	37498	2744900	P. L. Byard (1968), S. J. Wolnik et al. (1969), M. C. E. Huber & F. L. Tobey (1968), C. L. Cock, A. Stark & J. C. Evans (1973), M. C. E. Huber & R. J. Sandeman (1977), M. C. E. Huber, R. J. Sandeman & E. F. Tubbs (1975), S. M. Younger et al. (1978), G. A. Martin et al. (1988), R. L. Kurucz (1988)
Mn I	37983	1469883	D. E. Blackwell & B. S. Collins (1972), S. M. Younger et al. (1978), T. R. Greenlee & W. Whaling (1979), R. L. Kurucz (1988), G. A. Martin et al. (1988)
Fe I	37504	7498317	M. C. E. Huber & F. L. Tobey (1968), G. L. Grasdalen, M. Huber & W. H. Parkinson (1969), R. C. Hilborn & R. de Zafra (1973), W. Whaling et al. (1970), S. J. Wolnik, R. O. Berthel & G. W. Wares (1971), M. May, J. Richter & J. Wichelmann (1974), M. C. E. Huber (1974), F. P. Banfield & M. C. E. Huber (1973), J. M. Bridges & R. L. Kornblith (1974), H. Figger et al. (1975), D. E. Blackwell et al. (1979), J. R. Fuhr et al. (1988), R. L. Kurucz (1988)
Co I	23997	3752335	H. Figger et al. (1975), R. A. Roig & M. H. Miller (1979), J. R. Fuhr et al. (1981), J. R. Fuhr et al. (1988), R. L. Kurucz (1988)
Ni I	10061	732160	H. Heise (1974), R. B. King (1947b), J. R. Fuhr et al. (1988), R. L. Kurucz (1988), J. Laurent & S. Weniger (1970), W. N. Lennard et al. (1975), J. R. Fuhr et al. (1981), M. E. Wickliffe & J. E. Lawler (1997b)
Cu I	2178	32242	C. H. Corliss (1970), E. Biemont (1973), A. Bielski (1975)
Zn I	2212	129290	N. L. Moise (1966), B. Warner (1968a), A. A. Antena & V. A. Zilitis (1969), D. L. Lambert, E. A. Mallia & B. Warner (1969), T. Anderson & G. Sorensen (1973), R. Abjean & A. A. Johannin-Gilles (1975)
Sr I	1147	43222	C. H. Corliss & W. R. Bozman (1962)
Y I	3768	586984	C. H. Corliss & W. R. Bozman (1962), B. L. Cardon, W. H. Parkinson & F. S. Tomkins (1980), J. R. Fuhr et al. (1988)
Zr I	14107	5055470	C. H. Corliss & W. R. Bozman (1962), E. Biemont et al. (1981a)
Nb I	29578	7170524	C. H. Corliss & W. R. Bozman (1962), D. W. Duquette & J. E. Lawler (1982)
Mo I	38117	3123467	C. H. Corliss & W. R. Bozman (1962), S. E. Schenhage et al. (1983), W. Whaling et al. (1984) W. Whaling & J. W. Brault (1988),
Tc I	38320	5090717	
Ru I	36619	7421138	C. H. Corliss & W. R. Bozman (1962), E. Biemont et al. (1981b), S. Salih & J. E. Lawler (1985)
Rh I	24063	3035030	C. H. Corliss & W. R. Bozman (1962), M. Kwiatkowski et al. (1982), D. W. Duquette & J. E. Lawler (1985), S. Salih, D. W. Duquette & J. E. Lawler (1983)
Pd I	10229	571621	C. H. Corliss & W. R. Bozman (1962), E. Biemont et al. (1981c)
Ba I	1147	66443	C. H. Corliss & W. R. Bozman (1962), B. M. Miles & W. L. Wiese (1969)

Table 5. Count of states and transitionlines for each singly charged ion in the Kurucz database.

Element	$\mathtt{N}_{\mathtt{states}}$	$\mathtt{N}_{\mathtt{trans}}$	References
Be II	123	1418	W. L. Wiese et al. (1966), C. Laughlin (1978)
B II	763	34046	I. Martinson et al. (1970), J. Bromander (1971), A. Hibbert (1974), K. T. Cheng & W. R. Johnson (1977), C. Laughlin et al. (1978),
C II	1569	28924	W. L. Wiese et al. (1966), M. Druetta, M. C. Poulizac & J. Desequelles (1970), J. Bromander (1971), M. C. Poulizac, M. Druetta & P. Ceyzerat (1971), O. Sinanoglu (1973), R. P. McEachran & Cohen (1971), C. Laughlin & A. Dalgarno (1973), R. L. Kurucz & E. Peytremann (1975), R. D. Cowan, L. M. Hobbs & D. G. York (1982)
N II	3144	169232	J. B. Tatum (1968), W. L. Wiese et al. (1966), C. Nicolaides et al. (1971), P. D. Dumont et al. (1974), R. L. Kurucz & E. Peytremann (1975)
O II	3737	296883	W. L. Wiese et al. (1966), R. L. Kurucz & E. Peytremann (1975)
F II	4240	206549	W. L. Wiese et al. (1966), R. L. Kurucz & E. Peytremann (1975), E. H. Pinnington et al. (1976)
Ne II	1959	178364	W. L. Wiese et al. (1966), R. L. Kurucz & E. Peytremann (1975), A. V. Loginov & P. F. Gruzdev (1978a)
Na II	777	52696	R. L. Kurucz & E. Peytremann (1975)
Mg II	324	6018	J. H. Black, J. C. Wisheit & E. Laviana (1972), R. L. Kurucz & E. Peytremann (1975)
Al II	939	31420	B. Warner (1968a), W. L. Wiese et al. (1969), R. L. Kurucz & E. Peytremann (1975), A. W. Weiss (1975)
Si II	1764	36511	E. Schulz-Gulde (1969), W. L. Wiese et al. (1969), H. G. Berry et al. (1971), L. J. Curtis & W. H. Smith (1974), R. L. Kurucz & E. Peytremann (1975), M. C. Artru et al. (1981)
P II	3254	217038	W. L. Wiese et al. (1969), R. L. Kurucz & E. Peytremann (1975), M. H. Miller et al. (1971), A. Hibbert (1988)

Table 5 – *continued*

Element	$\mathrm{N}_{\mathtt{states}}$	$\mathrm{N}_{\mathtt{trans}}$	References
S II	2387	275137	R. L. Kurucz & E. Peytremann (1975), J. M. Bridges & W. L. Wiese (1967), H. G. Berry et al. (1970b), M. H. Miller et al. (1974), W. L. Wiese et al. (1969)
Cl II	3110	258102	W. L. Wiese et al. (1969), R. L. Kurucz & E. Peytremann (1975)
Ar II	2025	230953	W. L. Wiese et al. (1969), R. H. Garstang & H. Odabasi (1971), E. D. Tidwell (1972), B. F. W. Luyken (1972), R. L. Kurucz & E. Peytremann (1975), A. V. Loginov & P. F. Gruzdev (1978b),
K II	801	55355	H. G. Berry, J. Bromander & R. Buchta (1970a), R. L. Kurucz & E. Peytremann (1975)
Ca II	2884	115061	W. L. Wiese et al. (1969), J. H. Black et al. (1972), R. L. Kurucz (1988)
Sc II	1153	116491	W. L. Wiese & J. R. Fuhr (1975), R. L. Kurucz (1988), G. A. Martin et al. (1988)
Ti II	4414	897984	B. Warner (1967), S. J. Wolnik & R. O. Berthel (1973), J. R. Roberts, P. A. Voigt & A. Czernichowski (1975), W. L. Wiese & J. R. Fuhr (1975), R. L. Kurucz (1988), G. A. Martin et al. (1988)
V II	14162	4347545	B. Warner (1967), S. M. Younger et al. (1978), R. L. Kurucz (1988), G. A. Martin et al. (1988)
Cr II	29657	8683460	W. L. Shackleford (1965), B. Warner (1967), S. M. Younger et al. (1978), P. L. Byard (1968), R. L. Kurucz (1988), G. A. Martin et al. (1988)
Mn II	39503	5124343	R. L. Kurucz (1988), G. A. Martin et al. (1988)
Fe II	39418	7823961	J. R. Fuhr et al. (1988), R. L. Kurucz (1988)
Co II	38019	7951292	J. R. Fuhr et al. (1988), R. L. Kurucz (1988)
Ni II	21695	55833	H. Heise (1974), A. Goly, J. Moity & S. Weniger (1975), J. Moity (1978), R. L. Kurucz (1988), J. R. Fuhr et al. (1988)
Cu II	10061	584247	M. Kock & J. Richter (1968), R. L. Kurucz & E. Peytremann (1975)
Zn II	2212	968	S. R. Baumann & W. H. Smith (1970), T. Anderson & G. Sorensen (1973)
Sr II	296	5993	B. Warner (1968c)
Y II	1990	162441	C. R. Cowley & C. H. Corliss (1983), J. R. Fuhr et al. (1988)
Zr II	4021	1026414	E. Biemont et al. (1981a), C. R. Cowley & C. H. Corliss (1983)
Nb II	14110	15047	C. H. Corliss & W. R. Bozman (1962), P. Hannaford et al. (1985)
Mo II	29596	13272	C. H. Corliss & W. R. Bozman (1962), S. E. Schenhage et al. (1983)
Tc II	38246	119	
Ru II	38321	14670073	C. H. Corliss & W. R. Bozman (1962), W. F. Meggers, C. H. Corliss & C. H. Scribner (1975)
Rh II	36653	13817566	C. H. Corliss & W. R. Bozman (1962)
Pd II	24065	5191374	C. H. Corliss & W. R. Bozman (1962)
Ba II	119	1422	B. Warner (1968c), B. M. Miles & W. L. Wiese (1969)

Table 6. Data extracted from the NIST (A. Kramida et al. 2015; Y. Ralchenko & A. Kramida 2020; Y. Ralchenko 2024b) and Kurucz (R. L. Kurucz 2024, 2011) databases.

Database	Levels	Lines	Scope	Characteristic
NIST	94 neutral from H to Pa 91 singly charged from He to Pa	94 neutral from H to Pa 87 singly charged (He to Pa except Po, At, Rn, Fr)	General applications	Accurate
Kurucz	38 neutral and 37 singly charged	38 neutral and 37 singly charged	Hot stars	Complete

Table 7. Specification of the ExoMol file types. (Contents in brackets are optional.)

File Extension	File DSname	Contents
`.all`	Master	Single file defining contents of the ExoMol database.
`.def`	Definition	Defines contents of other files for each isotope.
`.states`	States	Energy levels, quantum numbers, uncertainties, lifetimes, (Landé g-factors).
`.trans`	Transitions	Einstein A coefficients (wavenumber).
`.broad`	Broadening	Parameters for pressure-dependent line profiles.
`.cross`	Cross sections	Temperature or temperature and pressure-dependent cross sections.
`.kcoef`	k-coefficients	Temperature and pressure-dependent k-coefficients.
`.pf`	Partition function	Temperature-dependent partition function.
`.cf`	Cooling function	Temperature-dependent cooling function.
`.cp`	Specific heat	Temperature-dependent specific heat.
`.super`	Super-lines	Temperature-dependent super-lines (histograms) on a wavenumber grid.
`.nm`	Vacuum-Ultraviolet (VUV) cross sections	Temperature and pressure-dependent VUV cross-sections (wavelength, nm).
`.fits`, `.h5`, `.kta`	Opacities	Temperature and pressure-dependent opacities for radiative-transfer applications.
`.overview`	Overview	Overview of data sets available.
`.readme`	Readme	Specifies data formats.
`.model`	Model	Specification of the spectroscopic model.

Table 8. Specification of the ExoAtom database file types.

File extension	$N_{\rm files}$	File DSname	Contents
.all	1	Master	Single file defining contents of the ExoAtom database
.adef.json	$N_{\rm iso}$	Definition	Defines contents of other files for each isotope
.states	$N_{\rm iso}$	States	Energy levels, quantum numbers, uncertainties, lifetimes, (Landé g-factors)
.trans	$N_{\rm iso}$	Transitions	Einstein A coefficients (wavenumber)
.pf	$N_{\rm iso}$	Partition Functions	Parameters for pressure-dependent line profiles

Note. $N_{\rm iso}$: total number of isotopes considered for each atom or ion (per data set).

Table 9. Source file for the value in `.trans` file of Kurucz database.

Source file name	Values contained
gfxxyy.lines	i, f
gfxxyy.agafgf	A, $\tilde{\nu}_{fi}$

Table 10. Source file for the value in `.states` file of Kurucz database.

Source file name	Contained Values
gfxxyy.gam	$\hat{E}$, J, g, Configuration, Term
lifexxyy.dat/gfxxyy.life	τ
Computed	i, g_J, Abbr

Table 9 shows which files from the Kurucz database are the source to form the ExoMol atomic `.trans` files, while Table 10 shows which files from the Kurucz database are the source to form the ExoMol atomic `.states` files. Although the Kurucz database contains several different files for transition lines, the NIST database provides more accurate data. To ensure a more complete data set, both predicted and measured lines from the Kurucz database are included. The `gfxxyy.lines` files are selected as they contain the majority of transition lines. However, the A coefficient and wavenumbers are not provided within the `.lines` files, for which we scraped the `.agafgf` files, which contain both values. The `lines` files do not have indices directly. Therefore, Energy, J, Configuration, and Term are matched to the `.states` file to retrieve the index.

To obtain the states data, there are only two files that hold the necessary values. One is `AELxxyy.DAT` and the other is `gfxxyy.gam`. However, the `AELxxyy.DAT` is now obsolete and contains less data than `.gam` files, which have all energy levels with J, QN, and g. Therefore, `gfxxyy.gam` was chosen to be scraped for the states. Lifetimes are stored in files `lifexxyy.dat` and `gfxxyy.life`, but the contents are the same. Uncertainties and state degeneracies, g_J, are not provided by the Kurucz database. Uncertainties for the Kurucz energy levels were arbitrarily set to 0.1 cm^{-1} and g_J calculated as $2J+1$.

For some species (Na I, K I, Ca II, Zn I, Y II), the Kurucz database provides three versions of the same file with different suffixes (w, y, z), but the data we scraped from all three files are identical. The Kurucz database also contains information on radiative, Stark, and Van der Waals damping for each species. These data are not included in the present version of ExoAtom.

In contrast to NIST, the Kurucz database provides partition functions in a single file, `partfnxxyy.dat`, which contains multiple partition function values under different potential lowering conditions, expressed in cm$^{-1}/Z^2_{\rm eff}$. These conditions are represented by column headers with values of -500, -1000, -2000, -4000, -8000, -16 000, and -32 000. However, there is no clear documentation of this or criterion for selecting the appropriate columns. Partition functions from the first column were chosen and were converted to the ExoMol format.

3.4 File naming convention

The file naming convention in the ExoAtom database ensures unique, descriptive, and machine-readable file names for each atom. The master file, named `ExoAtom.all.json`, defines the entire content of the ExoAtom database. All other files follow a standardized naming convention that applies to files with the `.adef.json`, `.states`, `.trans`, and `.pf` extensions. Each file name uses the format: `<atom_slug>__<database_name>`.

The atom slug is defined as follows. For neutral atoms, the element symbol is used; for singly charged atoms, the element symbol is appended with '`_p`'. Note that the NIST database has isotopically resolved data for the neutral hydrogen atom (H, D, T) and singly charged helium ion (^{3}He, ^{4}He) ion. For these two elements, the mass number is placed before the element symbol, for example '`2H`' and '`4He_p`'. There are no isotopically resolved data in the Kurucz database.

For example, the file name for a neutral iron atom from the NIST database is `Fe__NIST`, while the file name for a singly charged iron atom is `Fe_p__NIST`. Hydrogen has three isotopes in NIST: protium, deuterium, and tritium. Each isotope is named with its mass number as a superscript preceding the H. The corresponding file names are `1H__NIST`, `2H__NIST`, and `3H__NIST`, respectively.

3.5 Data format

3.5.1 The definition file

The ExoAtom database can be accessed at https://exomol.com/exoatom. The core information about each atomic species in the ExoAtom database is contained within its JSON definition file. JSON (JavaScript Object Notation) is a lightweight, human-readable format for data exchange that is commonly used to organize and transmit its structured scientific data (F. Pezoa et al. 2016).

The atomic definition file is called `adef.json` and adheres to the ExoAtom format `<AtomSlug>__<DataSetName>.adef.json`. This file specifies the available atomic data for a given species and describes potential applications, see Table 11. Appendix A presents the definition file `adef.json` for ^{1}H from the NIST data set as a typical example. These standardized fields allow consistent identification and reference across various isotopes. The purpose of this definition file is outlined as follows.

Standardized ExoAtom file usage The JSON structure follows a standardized format to ensure the identification for various atomic species. Each data set follows pre-defined fields that enable structured organization, facilitating efficient data retrieval and comparison.

Within this definition file, information is organized into clearly defined sections that detail specific atomic characteristics and

Table 11. Specification of the ExoAtom definition file.

Field	Description
Species information	
atom	Atomic symbol
ordinary_formula	Ordinary chemical formula
spectroscopic_notation	Spectroscopic notation
charge	Charge of the species
name	Name of the species
mass_in_Da	Molecular mass in Daltons (Da)
Isotope information	
iso_formula	Isotopic chemical formula
iso_name	Isotope name
mass	Isotopic mass in Daltons (Da)
spin	Nuclear spin value
atomic mass number	Mass number of the isotope
Data set information	
name	Data set name
version	Data set version (YYYYMMDD format)
doi	Digital Object Identifier for the data set
max_temperature	Maximum temperature in data set (K)
n_L_default	Default number of Lorentzian pressure-broadening parameters value
num_pressure_broadeners	Number of pressure broadeners
nxsec_files	Number of cross-section files
nkcoeff_files	Number of k-coefficient files
dipole_available	Availability of dipole data
cooling_function_available	Availability of cooling function data
specific_heat_available	Availability of specific heat data
Ionization	Ionization data (null if not available)
States information	
number_of_states	Total number of states
max_energy	Maximum energy in data set (cm^{-1})
uncertainty_available	Indicates if uncertainty is described
lifetime_available	Availability of lifetime data
lande_g_available	Availability of Landé g-factor
num_quanta	Number of quantum numbers
states_file_fields	List of fields in the states file, including:
ID	Unique integer identifier for the energy level
E	State energy in cm^{-1}
gtot	State degeneracy
J	Total angular momentum quantum number (integer/half-integer)
Unc	Uncertainty in the state energy in cm^{-1}
gfactor	Landé g-factor (optional)
qn:configuration	Configuration for the state
qn:LSCoupling	Term for the state
qn:parity	Parity for the state
Transitions information	
number_of_transitions	Total number of transitions
number_of_transition_files	Number of transition files
max_wavenumber	Maximum wavenumber (cm^{-1})
transitions_file_fields	List of fields in the transition file, including:
i	Upper state ID
f	Lower state ID
A	Einstein A coefficient (s^{-1})
Wavenumber	Transition wavenumber in cm^{-1}
Partition function	
max_partition_function_temperature	Maximum temperature for partition function (K)
partition_function_step_size	Step size for partition function (K)
fields	List of fields for the partition function, including:
T	Temperature in Kelvin
Q(T)	Partition function (dimensionless)

Table 12. Extract from the ExoAtom master file showing general atomic species (Fe and Fe^+).

Field	Description
exoatom.master	ID
20240601	Version number (format YYYYMMDD)
General atomic species (Iron)	
Atom name	Iron
Chemical formula	Fe
Number of isotopes	1
Data set name	NIST, Kurucz
Version number	20240601
Iron ion (II)	
Atom name	Iron Ion (II)
Chemical formula	Fe_p
Number of isotopes	1
Data set name	NIST, Kurucz
Version Number	20240601

spectroscopic properties. The general JSON structure includes sections for Species, and Data set (Data set information; States, Transitions, and Partition Functions files information).

Enhanced database functionality When isotopic data is provided for ExoAtom, the JSON file includes an additional Isotope section. This section describes the isotopic formula, isotope name, atomic mass, nuclear spin, and atomic mass number, see Table 11. Nuclear spin (I) describes the intrinsic angular momentum of atomic nuclei, determined by the pairing of protons and neutrons. Different isotopes of an element have different numbers of neutrons, which affects their nuclear spin values. The nuclear spin depends on the total number of protons and neutrons and follows specific rules. Including more complete isotope-resolved data and hyperfine-resolved transitions would enhance the database's precision.

Version control and data set updates Each data set is version-controlled, ensuring that users can track modifications and access the latest available data. The `version` field, formatted as `YYYYMMDD`, allows systematic updates without requiring manual intervention. This versioning mechanism supports seamless data integration and enhances the reliability of long-term scientific studies.

3.5.2 The master file

A summary file, named `exoatom.all.json`, consolidates the contents of the entire database. This file, which is available at www.exomol.com/exoatom/exoatom.all.json, provides a computer-readable (JSON format) list of recommended data sets, including those for each atomic species in the ExoAtom structure.

The master file summarizes the database's content and provides easy access to the latest version number of each data set, allowing users to track updates efficiently. It begins with general information about the database, including the total count of atomic species, isotopes, and data sets sourced from three different projects. Specifically, this database currently includes 151 atomic species from 2 databases.

Each atomic species in the ExoAtom master file is recorded separately, even if they correspond to a neutral atom and its ionized form. For example, iron (Fe) and its singly ionized state (Fe^+) are both treated as distinct entries, see Table 12. Each entry includes the chemical formula, number of isotopes considered, as well as data set sources and version numbers. This structure ensures that users can clearly distinguish between neutral atoms and their ionized states while maintaining consistency across data sets.

Table 13. Extract from the ExoAtom master file showing an atom with isotopes specified (hydrogen).

Field	Description
name	Hydrogen
formula	H
num_isotopes	3
isotopes	
iso_slug	`1H`, `2H`, `3H`
iso_formula	(1H), (2H), (3H)
data set	NIST
version	20240901

For elements with isotopic variations, each isotope is listed, as illustrated by hydrogen and its three isotopes three isotopes (^{1}H, ^{2}H, ^{3}H) given in Table 13. The master file provides detailed information, including the isotopic formula, data set source, and version number, see Appendix B.

Tables 12 and 13 illustrate the structured representation of atomic species in the master file. Table 12 presents general atomic species, using Fe and Fe^+ as examples, where both the neutral and ionized forms are recorded separately. Table 13 demonstrates an element with multiple isotopes, using hydrogen as an example, detailing its three isotopic variants (^{1}H, ^{2}H, and ^{3}H) along with their data set sources and version information.

3.5.3 States files

`.states` files consist of the index i, energy term value $\tilde{E}$ (cm^{-1}), the J-dependent state degeneracy g_J, quantum number J, uncertainty Unc (cm^{-1}), lifetime τ, Landé g-factor g, and state label QN (J. Tennyson et al. 2024).

For the ExoAtom database we have decided to follow the NIST convention and omit the nuclear spin degeneracy from g_J. This is different from the molecular ExoMol database which follows the HITRAN (R. R. Gamache et al. 2025) convention, which includes the nuclear spin degeneracy. This so-called physicist's convention is not adopted by ExoAtom since for nearly all atoms in the database the isotope is not specified (astrophysicist's convention; Y. V. Pavlenko et al. 2020) and hence the value of the nuclear spin is not specified either. This means that the degeneracy factor g_i is simply given by:

$$g_i = 2J_i + 1, \tag{1}$$

where J_i is the total angular momentum quantum number of i-th level.

In atomic spectroscopy, different coupling schemes describe how angular momenta combine to determine the total angular momentum $\vec{J}$. In ExoAtom, according to Y. Ralchenko (2024a), the LS coupling (Russell-Saunders coupling), jj coupling (individual total angular momentum coupling), and Racah symbols are selected as the term types for the NIST database. For the Kurucz database, while essentially based on the LS-coupling, much of the notation deviates from the standardized conventions typically used in spectroscopic databases. However, the original notation has been retained in its current form for the time being, with a potential revision considered as part of a future upgrade. Therefore, in all `JSON` files of the Kurucz database, the corresponding value for the term field is simply set to 'Kurucz'.

The LS coupling is used mostly in light atoms where the spin-orbit coupling is weak. First, the total orbital angular momentum $\vec{L}$ and total spin angular momentum $\vec{S}$ of all electrons couple, forming the total angular momentum $\vec{J} = \vec{L} + \vec{S}$. The resulting terms follow

Table 14. Specification of the ExoAtom `.states` file.

Field	Fortran format	C format	Description
ID	`I12`	`%12d`	State ID
$\tilde{E}$	`F12.6/` `F12.5/F12.4`	`%12.6f/` `%12.5f/%12.4f`	State energy in cm^{-1}
g_J	`I6`	`%6d`	State degeneracy
J	`I7/F7.1`	`%7d/%7.1f`	Total angular momentum quantum number, J (integer/half-integer)
Unc	`F12.6`	`%12.6f`	Uncertainty in the state energy in cm^{-1}
τ †	`ES12.4`	`%12.4e`	Radiative lifetime in s (optional, Kurucz only)
gfactor†	`F10.6`	`%10.6f`	Landé g-factor (optional, Kurucz only)
qn:configuration	`A12`	`%12s`	Configuration for the state
term	`A8`	`%8s`	Term for the state
qn:parity†	`A1`	`%1s`	Parity for the state (optional, NIST only)
Abbr†	`A2`	`%2s`	Abbreviation indicating data source: `CA` (calculated, Kurucz) or `NI` (measured, NIST)

Notes. The `.states` file typically contains 9–10 columns. Columns marked with † are optional, depending on the data source. The `.states` file is generated from the levels data using the following conversion rules:

(i) The ExoMol data standards use the given data formats for columns which should be separated by a single space.
(ii) ID: Integer, starts from 1 and ends with the number of valid rows in levels data.
(iii) $\tilde{E}$: Different formats apply: $\tilde{E} \leq 100000$: `F12.6` or `%12.6f`, $100000 \leq \tilde{E} < 1000000$: `F12.5` or `%12.5f`, $\tilde{E} \geq 1000000$: `F12.4` or `%12.4f`.
(iv) g_J: Obtained directly from g in the levels data. When the atom has isotopes, it corresponds to $g_{\rm tot}$; when atomic isotope is not specified, it corresponds to g_J.
(v) J: Obtained directly from J in levels data.
(vi) Unc: Obtained directly from Uncertainty (cm^{-1}) in levels data.
(vii) g: Obtained from Landé g-factor column in levels data. If this column is absent, it will not appear in the `.states` file.
(viii) qn:configuration: Directly from the configuration column in levels data. The format should follow the `pyvalem` program (https://github.com/xnx/pyvalem).
(ix) term: Directly from the term column in levels data. The trailing '$*$' should be removed if applicable. Format should be consistent with `pyvalem`.
(x) qn:parity: Terms of odd parity (those ending in $*$ in the original data sources) are marked with - in this field; those of even parity are marked with +.
(xi) Abbr: Only in Kurucz-based files; indicates whether the level is experimentally identified (`NI`) or purely calculated (`CA`).

Table 15. Extract from the `.states` file for NIST database for Li I (neutral lithium atom)

i	$\tilde{E}$	g_J	J	Unc	qn:configuration	term	qn:parity
1	0.000000	2	0.5	0.100000	1s2.2s	2S	+
2	14903.660000	2	0.5	0.100000	1s2.2p	2P	-
3	14904.000000	4	1.5	0.100000	1s2.2p	2P	-
4	27206.120000	2	0.5	0.100000	1s2.3s	2S	+
5	30925.380000	2	0.5	0.100000	1s2.3p	2P	-

the spectroscopic notation $^{2S+1}L_J$, where S represents the total spin multiplicity, $\vec{L}$ is the total orbital angular momentum (denoted by spectroscopic symbols such as $S, P, D, F, \ldots$), and $\vec{J}$ is the total angular momentum. In contrast, jj coupling is more appropriate for heavy atoms where spin-orbit interaction is strong. Here, each electron's individual orbital angular momentum $\vec{l}$ and spin $\vec{s}$ couple first to form $\vec{j} = \vec{l} + \vec{s}$, and then these $\vec{j}$ values combine to determine the total angular momentum $\vec{J}$ of the system. The resulting terms are written in terms of $\vec{j}$-values rather than $\vec{L}$ and $\vec{S}$, making this coupling more relevant for relativistic calculations. Racah symbols are used to further analyse angular momentum coupling. These symbols, denoted as $\langle j_1\, j_2 \mid j_3\, j_4 \rangle$, describe recoupling coefficients that simplify angular momentum calculations, such as Clebsch-Gordan and Racah coefficients.

Table 14 defines the specification of ExoAtom `.states` file both for data from NIST database and Kurucz database. It includes key spectroscopic parameters such as the state index, energy, degeneracy, total angular momentum J, uncertainty, Landé g-factor, lifetime, and relevant configuration or term labels. Tables 15 and 16 illustrates a representative sample (Li I) `.states` file from NIST database and Kurucz database, respectively. The value 'Abbr', see Table 10, is used for the Kurucz data to distinguish whether a state is predicted or not: predicted/calculated energies are labelled 'CA', while measure empirical energies taken from NIST, are labelled 'NI'; see L. K. McKemmish et al. (2024) for a discussion of these tags. Differences between the 'NI' levels in Kurucz and those listed in the NIST `.states` file arise because the Kurucz data set is a hybrid compilation that combines both observed and theoretical energies. Therefore, the retained NIST identifiers indicate the observational origin of the term assignment rather than ensuring identical numerical energy values.

3.5.4 *Trans files*

Similar to the `.states` file format, the ExoMol `.trans` format consists of upper state ID i, lower state ID f, Einstein A coefficient, and Transition wavenumber $\tilde{\nu}_{if}$, seen Table 17. Tables 18 and 19 illustrate a representative sample (Li I) `.trans` file from the NIST database and Kurucz database, respectively. As discussed above, for some atoms the associated `.trans` files could not be produced due to the absence of the Einstein coefficient or lack of the relevant description.

Table 16. Extract from the `.states` file for Kurucz database for Li I (neutral lithium atom).

i	$\tilde{E}$	g_J	J	Unc	τ	$g$factor	qn:Configuration	term	Abbr
33	40439.020000	8	3.5	0.100000	4.0323e-07	0.889000	1s2.6g	2G	NI
34	40439.070000	10	4.5	0.100000	6.0606e-07	0.909000	1s2.6h	2H	NI
35	40439.070000	12	5.5	0.100000	6.0606e-07	1.091000	1s2.6h	2H	NI
36	40967.990000	2	0.5	0.100000	2.7174e-07	2.002000	1s2.7s	2S	NI
37	41217.580000	2	0.5	0.100000	7.6336e-07	0.666000	1s2.7p	2P	NI

Note. Abbr: Abbreviation inherited from Kurucz metadata. `CA` denotes calculated levels, and `NI` indicates experimentally identified levels; values are retained from the Kurucz data set.

Table 17. Specification of the .trans file (J. Tennyson et al. 2024).

Field	Fortran format	C format	Description
i	I12	%12d	Upper state ID
f	I12	%12d	Lower state ID
A	ES12.6	%12.6e	Einstein A coefficient in s^{-1}
$\tilde{\nu}_{if}$	E15.6	%15.6e	Transition wavenumber in cm^{-1}

Notes. The .trans file contains 4 columns and is generated by combining data from the levels and lines data. Each valid row in the lines data corresponds to a row in the .trans file. The values for columns i and f are obtained from the levels data according to the following rules:

Table 18. Extract from the transitions file for NIST database for Li I (neutral lithium atom).

i	f	A	$\tilde{\nu}_{fi}$
15	13	6.900000E-02	6.800000E+00
14	13	4.600000E-03	6.800000E+00
14	12	6.440000E-02	6.800000E+00
21	19	6.500000E-01	9.600000E+00
21	20	4.640000E-02	9.600000E+00

Table 19. Extract from the transitions file for Kurucz database for Li I (neutral lithium atom).

i	f	A	$\tilde{\nu}_{fi}$
28	27	1.710000E+02	4.597000E+01
28	26	3.419800E+01	4.597000E+01
29	26	2.051200E+02	4.597400E+01
109	111	2.552700E+03	4.745000E+01
109	110	2.552700E+03	4.745000E+01
94	95	3.981100E+03	6.193000E+01

3.5.5 *Partition functions*

The partition functions for both NIST and Kurucz databases are provided separately, for reasons discussed below, as `.pf` files in standard ExoMol format. For NIST, the partition functions, $Q(T)$, were generated as a direct summation as given by:

$$Q(T) = \sum_i g_i e^{-\frac{c_2 \tilde{E}_i}{T}}, \tag{2}$$

where i, in principle, runs over all states in the system; $\tilde{E}_i$ is the corresponding energy term value in cm^{-1}, $c_2 = 1.438776877$ K/cm^{-1} is the second radiation constant, and T is the temperature in K. Finally, $g_i = 2J_i + 1$ is the degeneracy of state i, where we also follow the so-called astrophysicist's convention. Table 20 provides the format for the partition function (.pf) files.

It should be noted that there is an issue with the infinite number of bound levels in atoms that can lead to the partition function becoming infinite under some circumstances, see the discussion given by P. Alimohamadi & G. J. Ferland (2022). Given the different number of states provided by the NIST and Kurucz differ significantly, the two databases provide different approaches to this problem.

NIST provides partition functions at a given temperature computed as the direct sum over the tabulated energy levels. We mimicked this and tests showed that our partition functions agree well with those provided by NIST. Partition functions in NIST are therefore provided for each species on a 1 K grid up to 6000 K. Higher temperature partition functions can easily be computed using the program PyExoCross (J. Zhang et al. 2024).

In contrast, the Kurucz database explicitly provides partition functions, which we used directly. The temperature grid for the Kurucz partition functions is coarser than that used for the NIST data but given the slow variation in atomic partition functions with temperature should be sufficient for practical applications. Comparison between NIST and Kurucz values show them to be similar for simple systems but they can differ for systems with many low-lying excited states. Fig. 1 compares ExoAtom partition functions generated for NIST by PyExoCross with those directly scraped from the Kurucz database. We could see that these three match very well. The agreement between the representations of the partition function is good: the maximum difference over the entire temperature range considered is less than 0.2 per cent for Al, 0.1 per cent for Mg, and 0.1 per cent for Fe.

Tables 21 and 22 illustrate representative samples of `.pf` files for Li I from the NIST and Kurucz databases, respectively. Both columns represent the partition function values at different temperatures. However, in the NIST database, the temperature steps are fixed with an interval of 1 K, whereas in the Kurucz database, the temperature steps are non-uniform and vary across the data set.

4 POST-PROCESSING

PyExoCross (J. Zhang et al. 2024) is a Python package that uses ExoMol-formatted data to generate spectra, cross-sections, lifetimes and opacities. With PyExoCross, spectra can be plotted based on the ExoMol-formatted atomic `.states` and `.trans` files to facilitate comparison with existing plots and other purposes.

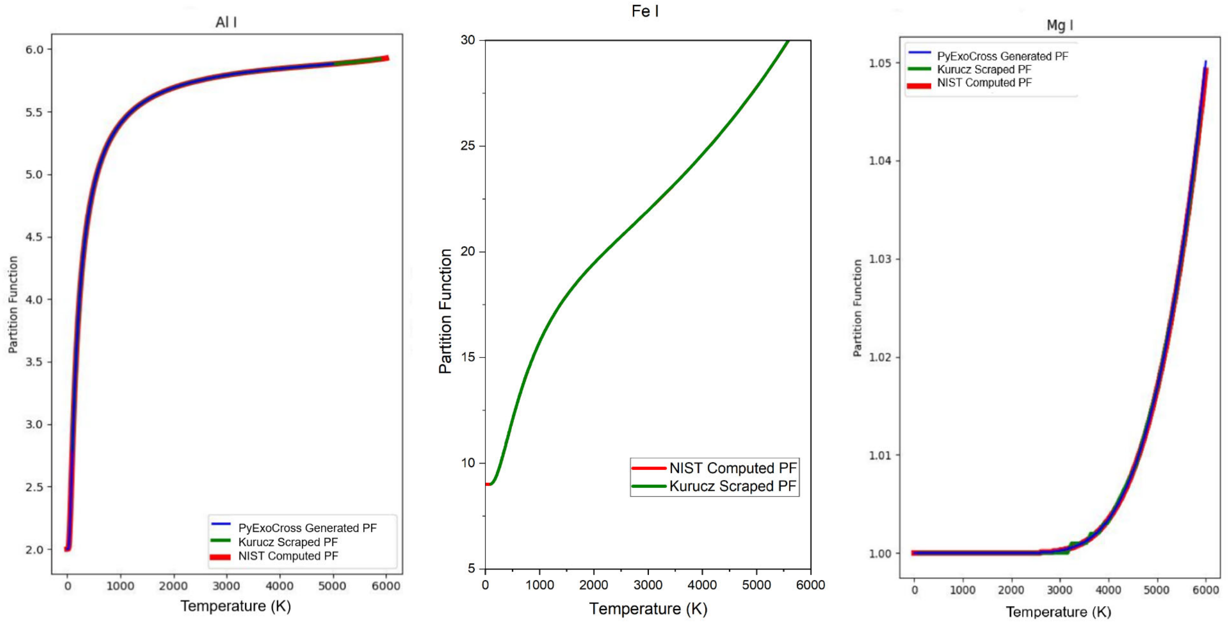

Figure 1. Comparison of partition functions for Al I, Fe I and Mg I, see the text for further details.

Table 20. Specification of the ExoMol format `.pf` file (source from partfnxxyy.dat file in Kurucz).

Field	Fortran Format	C Format	Description
T	F8.1	%8.1f	Temperature in K
$Q(T)$	F15.4	%15.4f	Partition function

Note. The individual columns should be separated by an a additional single space.

Table 21. Sample partition function calculation file from the .states file for Ca I (neutral calcium atom) in the NIST database.

T	$Q(T)$
5012.0	1.1737
5013.0	1.1739
5014.0	1.1741
5015.0	1.1743
5016.0	1.1744
5017.0	1.1746

Table 22. Sample partition function calculation file from the .states file for Ca I (neutral calcium atom) in the Kurucz database.

T	$Q(T)$
5012.0	1.1730
5129.0	1.1950
5248.0	1.2180
5370.0	1.2450
5495.0	1.2730
5623.0	1.3050

The use of PyExoCross to generate spectra is illustrated in Fig. 2, which presents emission spectra at temperatures of 3000 and 6000 K generated from the NIST and Kurucz line lists within ExoAtom. The emission spectra were computed using pure Doppler line broadening with a bin size of 0.0003 nm, without any collisional or pressure broadening. At 3000 K, both databases reproduce the key spectral features with good agreement for the peak position, while at 6000 K the more complete Kurucz database shows many more lines. There are also some differences for the predicted line cross sections.. For the NIST atomic database, uncertainties are provided for line positions (observed and Ritz wavelengths), but quantitative uncertainties for line cross sections are generally not reported; however the NIST data for Fe I are substantially taken from J. R. Fuhr et al. (1988) who in turn use the highly accurate measured oscillator strengths of D. E. Blackwell et al. (1982). Conversely the Kurucz data appears to be taken from R. C. Peterson & R. L. Kurucz (2014) who computed oscillator strengths using the R. D. Cowan (1981) code. These sorts of differences are a feature of our comparisons between the two sets of data; where lines exist in both codes, our assumption is the data provided by the NIST atomic database should be favoured. At high temperatures Kurucz contains many strong transitions that are not recorded in NIST.

5 CONCLUSIONS

The ExoAtom database extends the ExoMol framework by providing high-accuracy atomic spectral data in a standardized format. This database integrates energy levels, radiative transitions, and partition functions for a wide range of neutral and ionized atoms, primarily sourced from the NIST and Kurucz databases. By structuring atomic data in the ExoMol format, ExoAtom enhances accessibility and ensures compatibility with established atomic data sets.

The current version of ExoAtom includes line lists for 79 neutral and 71 singly ionized elements from the NIST database, as well as 38 neutral and 37 singly ionized elements from the Kurucz database. The NIST database provides highly accurate data, whereas the Kurucz database offers a more complete data set. Thus, ExoAtom does not recommend one data set over another but instead presents both to accommodate different research needs. These data sets play a crucial role in modelling atomic processes in astrophysical environments, including stellar atmospheres, exoplanetary spectra, and the interstellar medium. We note that while nearly all detections

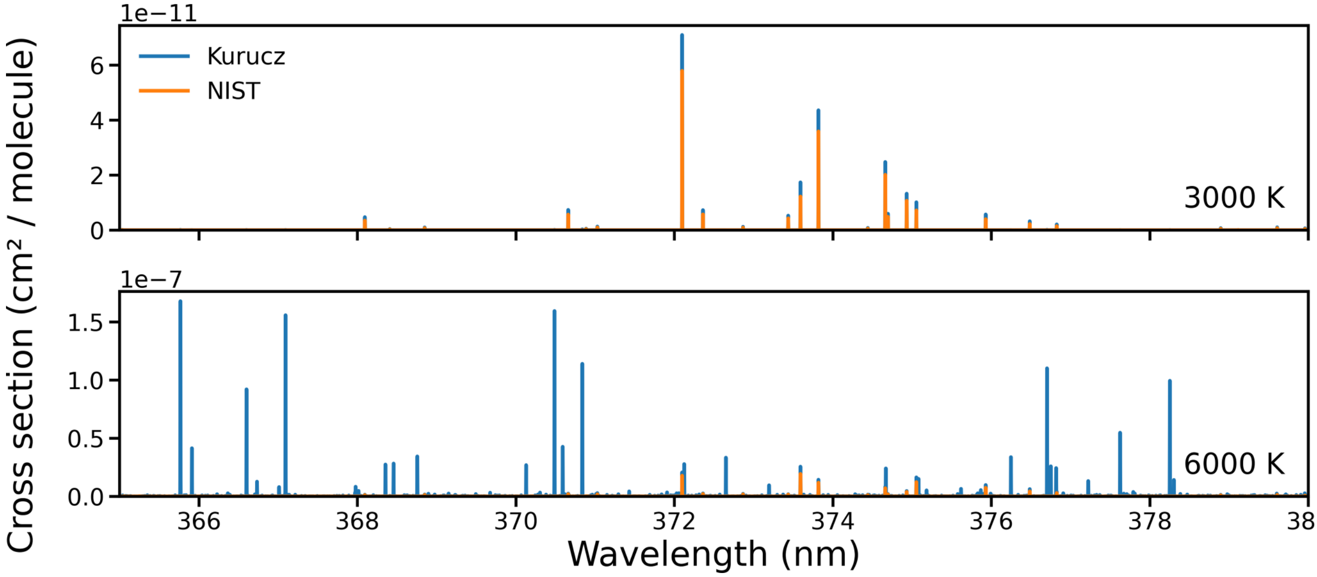

Figure 2. Comparison of NIST (Y. Ralchenko & A. Kramida 2020) and Kurucz (R. L. Kurucz 2018) Fe I emission spectra at 3000 K and 6000 K; the 6000 K spectrum contains many lines only present in the Kurucz data set.

of atoms in exoplanets involve neutral or singly ionized species, some studies have focused on more highly ionized atoms (J. L. Linsky et al. 2010). Therefore, our plan is to expand the ExoAtom database to include further ionization stages in due course. At present, the ExoAtom database has contains no line-broadening information. We note that the Kurucz database contains information on radiative, Stark and Van der Waals damping for most species, concentrating largely on measured lines. We plan to add line-broadening parameters for atoms and atomic ions in due course.

The ExoMol group welcomes collaborations and contributions from external sources to further enrich their databases including the ExoAtom database. The ExoAtom database https://exomol.com/exoatom/ is publicly available through the ExoMol website. We hope it will provide a valuable resource for spectroscopic modelling and interpreting observations.

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Since we started this project, Robert (Bob) Kurucz passed away on 2025 March 1 (see A. Dupree & C. Conroy (2025)) and the NIST Atomic Physics group has been closed. We wish to dedicate this paper to the talented atomic physicists whose work we make use of in this paper.

CONFLICT OF INTEREST

Authors declare no conflict of interest.

DATA AVAILABILITY

All the data discussed in this paper are freely available from the ExoAtom website https://exomol.com/exoatom.

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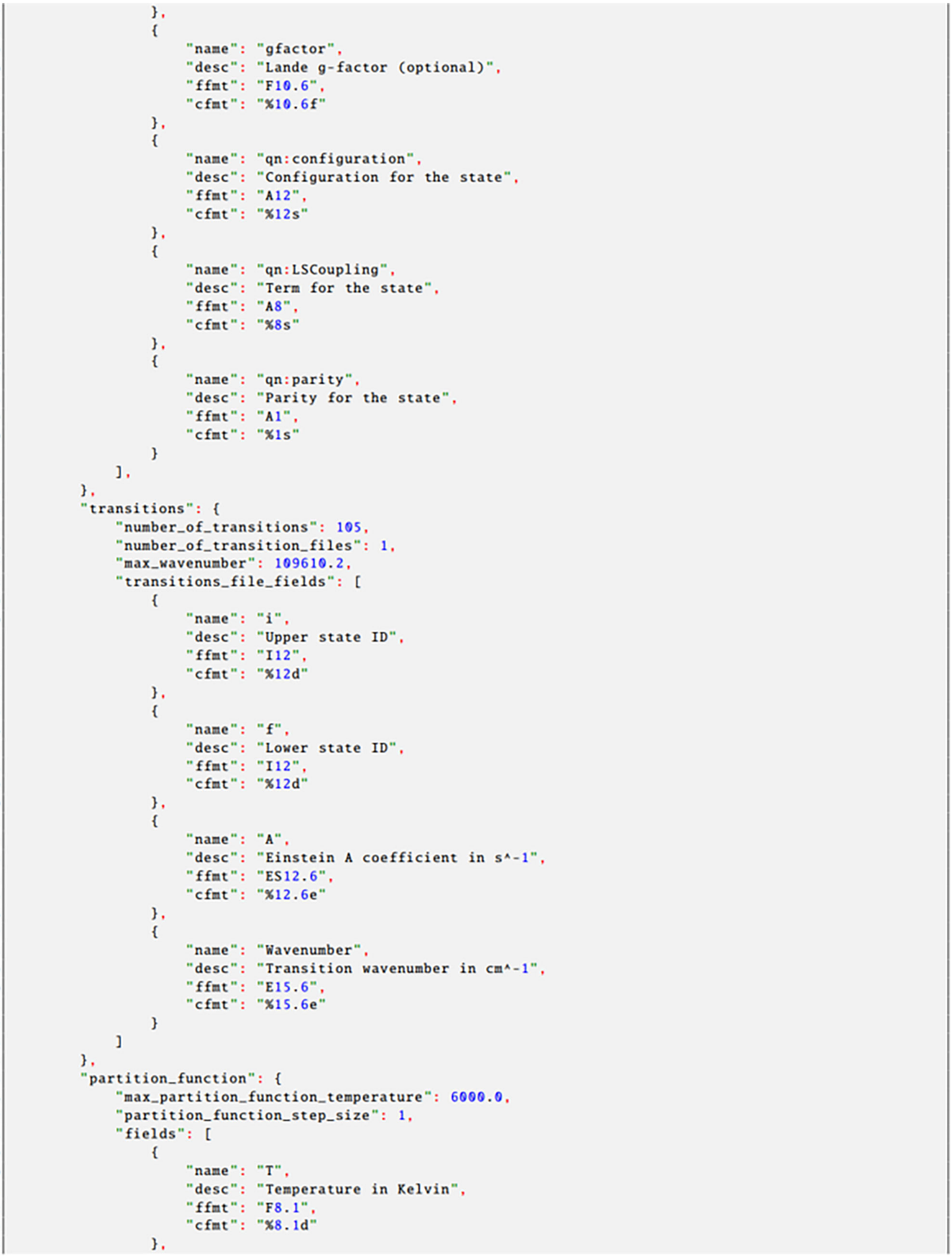
APPENDIX A: EXAMPLE `adef.json` FILE FOR THE H ATOM

```
{
    "species": {
        "atom": "H",
        "ordinary_formula": "H",
        "spectroscopic_notation": "H I",
        "charge": 0,
        "name": "hydrogen",
        "mass_in_Da": 1.00784
    },
    "isotope": {
        "iso_formula": "(1H)",
        "iso_name": "hydrogen",
        "mass": 1.00784,
        "spin": "1/2",
        "atomic mass number": 1
    },
    "dataset": {
        "name": "NIST",
        "version": 20240901,
        "doi": "",
        "max_temperature": 6000,
        "n_L_default": 0.5,
        "num_pressure_broadeners": 0,
        "nxsec_files": 0,
        "nkcoeff_files": 0,
        "dipole_available": false,
        "cooling_function_available": false,
        "specific_heat_available": false,
        "uncertainty_available": true
        "Ionisation": null,
        "states": {
            "number_of_states": 105,
            "max_energy": 109610.2232,
            "lifetime_available": false,
            "lande_g_available": false,
            "num_quanta": 1,
            "states_file_fields": [
                {
                    "name": "ID",
                    "desc": "Unique integer identifier for the energy level",
                    "ffmt": "I12",
                    "cfmt": "%12d"
                },
                {
                    "name": "E",
                    "desc": "State energy in cm^-1",
                    "ffmt": "F12.6",
                    "cfmt": "%12.6f"
                },
                {
                    "name": "gtot",
                    "desc": "State degeneracy",
                    "ffmt": "I6",
                    "cfmt": "%6d"
                },
                {
                    "name": "J",
                    "desc": "Total angular momentum quantum number, J (half-integer)",
                    "ffmt": "F7.1",
                    "cfmt": "%7.1f"
                },
                {
                    "name": "Unc",
                    "desc": "Uncertainty in the state energy in cm^-1",
                    "ffmt": "F12.6",
                    "cfmt": "%12.6f"
```



```
                },
                {
                    "name": "gfactor",
                    "desc": "Lande g-factor (optional)",
                    "ffmt": "F10.6",
                    "cfmt": "%10.6f"
                },
                {
                    "name": "qn:configuration",
                    "desc": "Configuration for the state",
                    "ffmt": "A12",
                    "cfmt": "%12s"
                },
                {
                    "name": "qn:LSCoupling",
                    "desc": "Term for the state",
                    "ffmt": "A8",
                    "cfmt": "%8s"
                },
                {
                    "name": "qn:parity",
                    "desc": "Parity for the state",
                    "ffmt": "A1",
                    "cfmt": "%1s"
                }
            ],
        },
        "transitions": {
            "number_of_transitions": 105,
            "number_of_transition_files": 1,
            "max_wavenumber": 109610.2,
            "transitions_file_fields": [
                {
                    "name": "i",
                    "desc": "Upper state ID",
                    "ffmt": "I12",
                    "cfmt": "%12d"
                },
                {
                    "name": "f",
                    "desc": "Lower state ID",
                    "ffmt": "I12",
                    "cfmt": "%12d"
                },
                {
                    "name": "A",
                    "desc": "Einstein A coefficient in s^-1",
                    "ffmt": "ES12.6",
                    "cfmt": "%12.6e"
                },
                {
                    "name": "Wavenumber",
                    "desc": "Transition wavenumber in cm^-1",
                    "ffmt": "E15.6",
                    "cfmt": "%15.6e"
                }
            ]
        },
        "partition_function": {
            "max_partition_function_temperature": 6000.0,
            "partition_function_step_size": 1,
            "fields": [
                {
                    "name": "T",
                    "desc": "Temperature in Kelvin",
                    "ffmt": "F8.1",
                    "cfmt": "%8.1d"
                },
```

```
                {
                    "name": "Q(T)",
                    "desc": "Partition function (dimensionless)",
                    "ffmt": "F15.4",
                    "cfmt": "%15.4d"
                }
            ]
        }
    }
}
```

APPENDIX B: EXTRACT FROM THE EXOATOM MASTER FILE SHOWING THE SPECIFICATIONS FOR THE H ISOTOPES, FE, AND FE ION

```
{
  "ExoAtom": {
    "ID": "exoatom.all.json",
    "version": 20240930
  },
  "atoms": [
    {
      "name": "Hydrogen",
      "formula": "H",
      "num_isotopes": 3,
      "isotopes": [
        {
          "iso_slug": "1H",
          "iso_formula": "(1H)",
          "dataset": "NIST",
          "version": 20240601
        },
        {
          "iso_slug": "2H",
          "iso_formula": "(2H)",
          "dataset": "NIST",
          "version": 20240601
        },
        {
          "iso_slug": "3H",
          "iso_formula": "(3H)",
          "dataset": "NIST",
          "version": 20240601
        }
      ]
    },
    {
      "name": "Iron",
      "formula": "Fe",
      "num_isotopes": 1,
      "isotopes": [
        {
          "iso_slug": "56Fe",
          "iso_formula": "(56Fe)",
          "dataset": "NIST",
          "version": 20240601
        },
        {
          "iso_slug": "56Fe",
          "iso_formula": "(56Fe)",
          "dataset": "Kurucz",
          "version": 20240115
        }
      ]
    },
    {
      "name": "Iron Ion (I)",
      "formula": "Fe_p",
      "num_isotopes": 1,
      "isotopes": [
        {
          "iso_slug": "56Fe_p",
          "iso_formula": "(56Fe_p)",
          "dataset": "NIST",
          "version": 20240601
        },
        {
          "iso_slug": "56Fe_p",
          "iso_formula": "(56Fe_p)",
          "dataset": "Kurucz",
```

```
            "version": 20240115
          }
        ]
      }
      // ... other atoms ...
    ]
}
```

This paper has been typeset from a TEX/LATEX file prepared by the author.