ExoAtom: A Database of Atomic Spectra in ExoMol Format

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ABSTRACT

We present the ExoAtom database, www.exomol.com/exoatom, 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

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Table 1. Data coverage of the ExoAtom database

Category	Atom Count	NIST	Kurucz
Neutral Atoms	80	79	38
Singly Charged Ions	74	71	37

1 INTRODUCTION

The ExoMol database was established in 2011 to provide molecular line lists for exoplanet and other atmospheres (Tennyson & Yurchenko 2012). Given their importance the ExoMol database included contributions due to atomic sodium (Allard et al. 2019) and potassium (Allard et al. 2016) in its opacity tables (Chubb et al. 2021). However, spectra of many neutral and singly ionised atoms are a regular feature of high resolution studies of exoplanetary atmospheres (Linsky et al. 2010; Fossati et al. 2010; Spake et al. 2018; Hoeijmakers et al. 2019, 2020, 2024; Jiang et al. 2023; Pelletier et al. 2023; D'Arpa et al. 2024; Simonnin et al. 2024). For example, Prinoth et al. (2025) considered the spectra of 89 neutral or singly ionised 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 (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 (Ralchenko & Kramida 2020) (henceforth simply NIST), the line list compilations due to Kurucz (2011, 2018), VALD3 (the third edition of the Vienna Atomic Line Database) (Ryabchikova et al. 2015), CHIANTI - An Atomic Database for Emission Lines (Del Zanna et al. 2021) and the Opacity Project (Seaton 2005) including the more focused spin-off Iron Project (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. Table 2 and Table 3 list the total number of energy states and transition lines for each atom and ion, respectively, in the NIST dataset. Table 4 and Table 5 provide the corresponding counts of states and lines for each atom and ion in the Kurucz database.

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	Kramida (2010), Jitrik & Bunge (2005)
^{2}H I	77	161	Kramida (2010), Wiese & Fuhr (2009)
^{3}H I	9	11	Kramida (2010), Wiese & Fuhr (2009)
^{4}He I	842	2289	Kandula et al. (2010), Wiese & Fuhr (2009)
Li I	181	257	Kelly (1987), Wiese & Fuhr (2009)
Be I	212	394	Cook et al. (2020), Fuhr & Wiese (2010)
B I	118	242	Kramida & Ryabtsev (2007), Fuhr & Wiese (2010)
C I	433	1616	Haris & Kramida (2017), Wiese & Fuhr (2007)
N I	366	1287	Pachucki (2024), Wiese & Fuhr (2007)
O I	580	854	Wiese et al. (1996), Demirdak et al. (2023)
F I	302	120	Pachucki (2024), Musielok et al. (1999)
Ne I	374	533	Seaton (1998), Saloman & Sansonetti (2005)
Na I	423	523	Sansonetti (2008a), Kelleher & Podobedova (2008a)
Mg I	303	1090	Kelleher & Podobedova (2008a), Martin & Zalubas (1980)
Al I	185	293	Kelleher & Podobedova (2008a), Martin & Zalubas (1979)
Si I	406	603	Kelleher & Podobedova (2008c), Martin & Zalubas (1983)
P I	284	132	Wiese et al. (1969), Martin et al. (1985)
S I	377	913	Podobedova et al. (2009), Martin et al. (1990)

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Table 2 – continued from previous page

Element	N_{state}	N_{trans}	References
Cl I	366	99	Wiese et al. (1969), Radziemski & Kaufman (1969)
Ar I	503	428	Fuhr & Wiese (1996),Minnhagen (1973)
K I	296	211	Wiese et al. (1969), Sansonetti (2008b)
Ca I	780	136	Wiese et al. (1969), Sugar & Corliss (1985)
Sc I	355	257	Martin et al. (1988), Sugar & Corliss (1985)
Ti I	558	496	Martin et al. (1988), Saloman (2012a)
V I	548	1162	Saloman & Kramida (2017b)
Cr I	618	522	Martin et al. (1988), Saloman (2012b)
Mn I	536	489	Martin et al. (1988), Sugar & Corliss (1985)
Fe I	837	2542	Fuhr & Wiese (2006), Nave et al. (1994)
Co I	277	336	Fuhr et al. (1988), Sugar & Corliss (1985)
Ni I	287	522	Fuhr et al. (1988), Litzén et al. (1993)
Cu I	360	37	Morton (2003), Sugar & Musgrove (1990)
Zn I	374	16	Morton (2003), Sugar & Musgrove (1995)
Ga I	257	23	Morton (2003), Shirai et al. (2007)
Ge I	618	26	Wiese & Martin (1980), Sugar & Musgrove (1993)
As I	84	14	Wiese & Martin (1989), Kelly (1987)
Br I	264	54	Wujec et al. (1999), Humphreys et al. (1971)
Kr I	527	184	Morton (2000), Saloman (2007)
Rb I	239	40	Sansonetti (2006)
Sr I	377	86	Sansonetti & Nave (2010)
Y I	176	189	Shang et al. (2015), Gil & Gonzalez (2017)
Mo I	281	498	Whaling & Brault (1988), Sugar & Musgrove (1988)
Tc I	274	13	Sansonetti & Martin (2005), Palmeri & Wyart (1999)
Ru I	228	11	Sansonetti & Martin (2005), Callender et al. (1988)
Rh I	75	111	Fuhr & Wiese (2005), Callender et al. (1988)
Pd I	143	8	Sansonetti & Martin (2005), Engleman et al. (1998)
Ag I	104	7	Wiese & Martin (1980), Badr et al. (2006)
Cd I	126	18	Wiese & Martin (1980), Vidolova-Angelova et al. (1996)
In I	111	27	Morton (2000), Karlsson & Litzén (2001)
Sn I	218	55	Wiese & Martin (1980), Brown et al. (1977)
Sb I	145	10	Sansonetti & Martin (2005), Hassini et al. (1988)
Te I	119	6	Morton (2000), Makdisi & Bhatia (1982)
I I	220	5	Sansonetti & Martin (2005), Cerny et al. (1991)
Xe I	443	187	Morton (2000), Saloman (2004)
Cs I	178	42	Sansonetti (2009)
Ba I	355	109	Wiese & Martin (1980),Curry (2004)
La I	206	279	Den Hartog et al. (2015), Martin et al. (2023)
Ce I	354	54	Lawler et al. (2010), Martin et al. (2023)
Nd I	229	4	Sansonetti & Martin (2005), Martin et al. (2023)
Sm I	220	7	Sansonetti & Martin (2005), Martin et al. (2023)
Eu I	316	142	Morton (2000), Martin et al. (2023)
Gd I	465	16	Sansonetti & Martin (2005), Martin et al. (2023)
Dy I	302	40	Wiese & Martin (1980), Sansonetti & Martin (2005)
Ho I	201	12	Sansonetti & Martin (2005), Martin et al. (2023)
Er I	313	10	Sansonetti & Martin (2005), Martin et al. (2023)
Tm I	477	349	Wickliffe & Lawler (1997a), Martin et al. (2023)
Yb I	182	5	Sansonetti & Martin (2005), Martin et al. (2023)
Lu I	198	44	Fedchak et al. (2000), Vergès & Wyart (1978)
Hf I	278	187	Duquette et al. (1986), Lawler et al. (2022)
Ta I	122	135	Fivet et al. (2006a), Martin et al. (2023)
W I	144	121	Kramida & Shirai (2006)
Ir I	53	37	Xu et al. (2007), Martin et al. (2023)
Pt I	184	166	Den Hartog et al. (2005), Blaise et al. (1992)
Au I	61	20	Fivet et al. (2006b), Sansonetti & Martin (2005)
Hg I	294	53	Fuhr & Wiese (2005), Saloman (2006)
Tl I	66	9	Wiese & Martin (1980), Martin et al. (2023)
Pb I	134	28	Morton (2000), Wood & Andrew (1968)

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Element	$N_{\rm state}$	$N_{\rm trans}$	References
Bi I	71	39	Werbowy & Kwela (2009), Wahlgren et al. (2001)
Fr I	122	149	Fuhr & Wiese (2005), Sansonetti (2007)
Ra I	81	19	Trimble et al. (2009), Dammalapati et al. (2016)
Ac I	52	91	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	Wiese & Fuhr (2009), Yerokhin & Shabaev (2015)
^{4}He II	148	140	Jitrik & Bunge (2005), Yerokhin & Shabaev (2015)
Li II	178	564	Wiese & Fuhr (2009), Drake (1988)
Be II	249	149	Fuhr & Wiese (2010), Kramida (2005)
B II	156	435	Fuhr & Wiese (2010), Ryabtsev et al. (2005)
C II	414	1433	Kramida & Haris (2022)
N II	178	786	Musielok et al. (1996), Sun et al. (2021)
O II	275	876	Wiese et al. (1996), Gil & Gonzalez (2017)
F II	290	67	Wiese et al. (1966), Kelly (1987)
Ne II	380	233	Wiese et al. (1966), Kramida & Nave (2008)
Na II	162	176	Kelleher & Podobedova (2008a), Sansonetti (2008a)
Mg II	137	482	Martin & Zalubas (1980), Kelleher & Podobedova (2008a)
Al II	217	986	Kelleher & Podobedova (2008b), Martin & Zalubas (1979)
Si II	148	474	Kelleher & Podobedova (2008c), Martin & Zalubas (1983)
P II	160	73	Wiese et al. (1969), Martin et al. (1985)
S II	232	753	Podobedova et al. (2009), Martin et al. (1990)
Cl II	274	221	Wiese et al. (1969), Radziemski & Kaufman (1974)
Ar II	418	307	Wiese et al. (1969), Saloman (2010)
K II	96	252	Sansonetti (2008b)
Ca II	71	99	Wiese et al. (1969), Sugar & Corliss (1985)
Sc II	168	139	Martin et al. (1988), Sugar & Corliss (1985)
Ti II	252	470	Martin et al. (1988), Saloman (2012a)
V II	407	1884	Saloman & Kramida (2017a)
Cr II	913	92	Morton (2003), Sugar & Corliss (1985)
Mn II	514	840	Kramida & Sansonetti (2013)
Fe II	1027	7293	Fuhr & Wiese (2006), Nave & Johansson (2012)
Co II	478	2746	Raassen et al. (1998), Sugar & Corliss (1985)
Ni II	713	208	Fuhr et al. (1988), Sugar & Corliss (1985)
Cu II	467	553	Kramida et al. (2017)
Zn II	93	22	Morton (2003), Sugar & Musgrove (1995)
Ga II	95	10	Shirai et al. (2007)
Ge II	127	20	Wiese & Martin (1980), Sugar & Musgrove (1993)
Kr II	162	20	Fuhr & Wiese (2005), Saloman (2007)
Rb II	165	49	Sansonetti (2006)
Sr II	70	33	Sansonetti (2012)
Y II	235	66	Hannaford et al. (1982), Nilsson et al. (1991)
Tc II	33	6	Sansonetti & Martin (2005), Gil & Gonzalez (2017)
Ru II	225	8	Sansonetti & Martin (2005), Karlsson et al. (2002)
Pd II	185	10	Sansonetti & Martin (2005), Lundberg et al. (2001)
Ag II	99	236	Kramida (2013b)
Cd II	95	87	Xu et al. (2004), Gil & Gonzalez (2017)
In II	194	528	Kramida (2013a)
Sn II	76	134	Haris et al. (2014)
Sb II	109	2	Sansonetti & Martin (2005), Gil & Gonzalez (2017)
Xe II	161	22	Fuhr & Wiese (2005), Saloman (2004)
Cs II	315	2	Sansonetti (2009)
Ba II	161	83	Wiese & Martin (1980), Curry (2004)

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Table 3 – continued from previous page

Element	N_{state}	N_{trans}	References
La II	109	84	Lawler et al. (2001), Güzelçimen et al. (2018)
Ce II	480	283	Lawler et al. (2009), Safronova et al. (2015)
Pr II	111	101	Li et al. (2007), Radžiūtė et al. (2020)
Nd II	325	99	Den Hartog et al. (2003), Radžiūtė et al. (2020)
Sm II	127	7	Sansonetti & Martin (2005), Radžiūtė et al. (2020)
Eu II	57	13	Sansonetti & Martin (2005), Radžiūtė et al. (2020)
Tb II	62	8	Sansonetti & Martin (2005)
Dy II	300	17	Sansonetti & Martin (2005)
Ho II	31	4	Sansonetti & Martin (2005), Radžiūtė et al. (2021)
Er II	111	7	Sansonetti & Martin (2005), Radžiūtė et al. (2021)
Tm II	351	13	Sansonetti & Martin (2005), Radžiūtė et al. (2021)
Yb II	284	10	Sansonetti & Martin (2005), Radžiūtė et al. (2021)
Lu II	37	9	Sansonetti & Martin (2005), Kahl et al. (2019)
Hf II	106	2	Sansonetti & Martin (2005), Allehabi et al. (2022)
W II	58	71	Kramida & Shirai (2006)
Ir II	53	126	Xu et al. (2007), van Kleef & Metsch (1978)
Pt II	277	183	Quinet et al. (2008), Wyart et al. (1995)
Hg II	114	446	Sansonetti & Martin (2005), Sansonetti & Reader (2001)
Tl II	76	3	Sansonetti & Martin (2005)
Pb II	90	3	Sansonetti & Martin (2005)
Bi II	77	4	Sansonetti & Martin (2005), Dolk et al. (2002)
Ra II	36	9	Sahoo et al. (2009), Dammalapati et al. (2016)
Ac II	83	288	Kramida (2022)

Table 4. $N_{\rm state}$ and $N_{\rm trans}$ for each Neutral in Kurucz Database (Kurucz 2014; Kurucz et al. 2009; Castelli & Kurucz 2010; Peterson & Kurucz 2014, 2022; Kurucz 2002; Castelli et al. 2015)

Element	$N_{\rm state}$	$N_{\rm trans}$	References
Li I	123	1424	Caves (1975); Lindgard & Nielsen (1977); Wiese et al. (1966); Sengupta (1975)
Be I	663	23574	Laughlin et al. (1978); Laughlin & Victor (1974); Wiese et al. (1966); Pfennig et al. (1965)
B I	1549	22012	Bromander (1971); Kurucz & Peytremann (1975); Martinson et al. (1970); Wiese et al. (1966)
C I	3500	250828	Bromander et al. (1978); Bromander (1971); Brooks et al. (1977); Cohen & McEachran (1978); Goly (1976); Kurucz & Peytremann (1975); Lambert (1968); Morton & Smith (1973); Miller et al. (1974); Wiese et al. (1966); Nussbaumer & Rusca (1979); Smith & Wiese (1971); Stuck & Wende (1974); Wiese et al. (1996)
N I	4479	356876	Brooks et al. (1977); Dumont et al. (1974); Kurucz & Peytremann (1975); Wiese et al. (1966); Nicolaides et al. (1971); Wiese et al. (1996)
O I	3932	109396	Bromander et al. (1978); Kurucz & Peytremann (1975); Wiese et al. (1966, 1996)
F I	1959	131375	Kurucz & Peytremann (1975)
Ne I	777	15361	Bengston & Miller (1970); Kurucz & Peytremann (1975); Lilly (1975,?); Martin & Campos (1977, 1978, 1979)
Na I	3131	51288	Kurucz & Peytremann (1975); Lindgard & Nielsen (1977); Wiese et al. (1969)
Mg I	588	22612	Anderson et al. (1967); Froese Fischer (1975a,b); Friedrich & Trefftz (1970); Kurucz (1975); Kurucz & Peytremann (1975); Laughlin & Victor (1974); Lincke & Ziegenbein (1971); Wiese et al. (1969); Schaefer (1971); Smith & Liszt (1971); Warner (1968b)
Al I	1888	29081	Kurucz (1975); Kurucz & Peytremann (1975); Lombardi et al. (1981); Wiese et al. (1969); Roig (1975); Smith & Liszt (1971)
Si I	3177	171085	Garz (1973); Grevess & Swings (1972); Kurucz (1975); Kurucz & Peytremann (1975); Miller (1968); Schulz-Gulde (1969)
P I	2387	202300	Kurucz & Peytremann (1975); Lawrence (1967); Livingston et al. (1975); Miller et al. (1971); Wiese et al. (1969)
S I	4171	13026	Foster (1967); Kurucz & Peytremann (1975); Wiese et al. (1969)
Cl I	1727	255821	Kurucz & Peytremann (1975)
Ar I	801	49824	Anisimove & Semenov (1974); Desai & Corcoran (1968); Kurucz & Peytremann (1975); Lilly (1976); Wiese et al. (1969); Woodyard & Altick (1979)
K I	2865	88919	Kurucz & Peytremann (1975); Mazing & Serapinas (1969); Wiese et al. (1969)
Ca I	1127	46062	Warner (1968a); Kurucz (1988); Wiese et al. (1969); Newsom (1966, 1968)
Sc I	4307	724611	Parkinson et al. (1976); Kurucz (1988); Martin et al. (1988); Wiese & Fuhr (1975)
Ti I	13977	5071484	Kurucz (1988); Klemt (1973); Lotrian et al. (1975); Martin et al. (1988); Wiese & Fuhr (1975); Smith & Kuhne (1978); Wolnik & Berthel (1973)
V I	29719	7056409	Kurucz (1988); King (1947a); Martin et al. (1988)
Cr I	37498	2744900	Byard (1968); Cock et al. (1973); Huber & Sandeman (1977); Huber et al. (1975); Huber & Tobey (1968); Kurucz (1988); Martin et al. (1988); Younger et al. (1978); Wolnik et al. (1969)
Mn I	37983	1469883	Blackwell & Collins (1972); Greenlee & Whaling (1979); Kurucz (1988); Martin et al. (1988); Younger et al. (1978)
Fe I	37504	7498317	Banfield & Huber (1973); Blackwell et al. (1979); Bridges & Kornblith (1974); Figger et al. (1975); Fuhr et al. (1988); Grasdalen et al. (1969); Huber & Tobey (1968); Huber (1974); Hilborn & de Zafra (1973); Kurucz (1988); May et al. (1974); Wolnik et al. (1971); Whaling et al. (1970)
Co I	23997	3752335	Figger et al. (1975); Fuhr et al. (1988); Kurucz (1988); Fuhr et al. (1981); Roig & Miller (1979)
Ni I	10061	732160	Fuhr et al. (1988); Heise (1974); Kurucz (1988); King (1947b); Laurent & Weniger (1970); Lennard et al. (1975); Fuhr et al. (1981); Wickliffe & Lawler (1997b)
Cu I	2178	32242	Bielski (1975); Biemont (1973); Corliss (1970)
Zn I	2212	129290	Abjean & Johannin-Gilles (1975); Anderson & Sorensen (1973); Antena & Zilitis (1969); Lambert et al. (1969); Moise (1966); Warner (1968a)
Sr I	1147	43222	Corliss & Bozman (1962)
Y I	3768	586984	Corliss & Bozman (1962); Cardon et al. (1980); Fuhr et al. (1988)
Zr I	14107	5055470	Biemont et al. (1981a); Corliss & Bozman (1962)
Nb I	29578	7170524	Corliss & Bozman (1962); Duquette & Lawler (1982)
Mo I	38117	3123467	Corliss & Bozman (1962); Schenhage et al. (1983); Whaling & Brault (1988); Whaling et al. (1984)
Tc I	38320	5090717	
Ru I	36619	7421138	Biemont et al. (1981b); Corliss & Bozman (1962); Salih & Lawler (1985)
Rh I	24063	3035030	Corliss & Bozman (1962); Duquette & Lawler (1985); Kwiatkowski et al. (1982); Salih et al. (1983)
Pd I	10229	571621	Biemont et al. (1981c); Corliss & Bozman (1962)
Ba I	1147	66443	Corliss & Bozman (1962); Miles & Wiese (1969)

3 DATABASE STRUCTURE

The Django web framework is used for the database implementation of ExoAtom, written in the Python programming language (Holovaty et al. 2003). The ExoAtom data structure is an extension of the original ExoMol data structure (Tennyson et al. 2013, 2024), see 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 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

Table 5. Count of States and Transition Lines for each Singly Charged Ion in Kurucz Database

Element	N_states	N_trans	References
Be II	123	1418	Laughlin (1978); Wiese et al. (1966)
B II	763	34046	Bromander (1971); Cheng & Johnson (1977); Hibbert (1974); Laughlin et al. (1978); Martinson et al. (1970)
C II	1569	28924	Bromander (1971); Cowan et al. (1982); Druetta et al. (1970); Kurucz & Peytremann (1975); Laughlin & Dalgarno (1973); McEachran & Cohen (1971); Wiese et al. (1966); Poulizac et al. (1971); Sinanoglu (1973)
N II	3144	169232	Dumont et al. (1974); Kurucz & Peytremann (1975); Wiese et al. (1966); Nicolaides et al. (1971); Tatum (1968)
O II	3737	296883	Kurucz & Peytremann (1975); Wiese et al. (1966)
F II	4240	206549	Kurucz & Peytremann (1975); Wiese et al. (1966); Pinnington et al. (1976)
Ne II	1959	178364	Kurucz & Peytremann (1975); Loginov & Gruzdev (1978a); Wiese et al. (1966)
Na II	777	52696	Kurucz & Peytremann (1975)
Mg II	324	6018	Black et al. (1972); Kurucz & Peytremann (1975)
Al II	939	31420	Warner (1968a); Kurucz & Peytremann (1975); Wiese et al. (1969); Weiss (1975)
Si II	1764	36511	Artru et al. (1981); Berry et al. (1971); Curtis & Smith (1974); Kurucz & Peytremann (1975); Wiese et al. (1969); Schulz-Gulde (1969)
P II	3254	217038	Hibbert (1988); Kurucz & Peytremann (1975); Miller et al. (1971); Wiese et al. (1969)
S II	2387	275137	Berry et al. (1970b); Bridges & Wiese (1967); Kurucz & Peytremann (1975); Miller et al. (1974); Wiese et al. (1969)
Cl II	3110	258102	Kurucz & Peytremann (1975); Wiese et al. (1969)
Ar II	2025	230953	Garstang & Odabasi (1971); Kurucz & Peytremann (1975); Luyken (1972); Loginov & Gruzdev (1978b); Wiese et al. (1969); Tidwell (1972)
K II	801	55355	Berry et al. (1970a); Kurucz & Peytremann (1975)
Ca II	2884	115061	Black et al. (1972); Kurucz (1988); Wiese et al. (1969)
Sc II	1153	116491	Kurucz (1988); Martin et al. (1988); Wiese & Fuhr (1975)
Ti II	4414	897984	Warner (1967); Kurucz (1988); Martin et al. (1988); Wiese & Fuhr (1975); Roberts et al. (1975); Wolnik & Berthel (1973)
V II	14162	4347545	Warner (1967); Kurucz (1988); Martin et al. (1988); Younger et al. (1978)
Cr II	29657	8683460	Byard (1968); Warner (1967); Kurucz (1988); Martin et al. (1988); Younger et al. (1978); Shackleford (1965)
Mn II	39503	5124343	Kurucz (1988); Martin et al. (1988)
Fe II	39418	7823961	Fuhr et al. (1988); Kurucz (1988)
Co II	38019	7951292	Fuhr et al. (1988); Kurucz (1988)
Ni II	21695	55833	Fuhr et al. (1988); Goly et al. (1975); Heise (1974); Kurucz (1988); Moity (1978)
Cu II	10061	584247	Kurucz & Peytremann (1975); Kock & Richter (1968)
Zn II	2212	968	Anderson & Sorensen (1973); Baumann & Smith (1970)
Sr II	296	5993	Warner (1968c)
Y II	1990	162441	Cowley & Corliss (1983); Fuhr et al. (1988)
Zr II	4021	1026414	Biemont et al. (1981a); Cowley & Corliss (1983)
Nb II	14110	15047	Corliss & Bozman (1962); Hannaford et al. (1985)
Mo II	29596	13272	Corliss & Bozman (1962); Schenhage et al. (1983)
Tc II	38246	119	
Ru II	38321	14670073	Corliss & Bozman (1962); Meggers et al. (1975)
Rh II	36653	13817566	Corliss & Bozman (1962)
Pd II	24065	5191374	Corliss & Bozman (1962)
Ba II	119	1422	Miles & Wiese (1969); Warner (1968c)

Table 6. Data Extracted from NIST (Ralchenko & Kramida 2020; Ralchenko 2024b; Kramida et al. 2015) and Kurucz (Kurucz 2024, 2011) Databases.

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

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 datasets 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 dataset 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

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 datasets 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

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

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 (Ralchenko & Kramida 2020; Ralchenko 2024b; Kramida et al. 2015), and the data were scraped by 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 is 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 datasets. 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 dataset, using the formula Unc = 2×10^{-N} 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.

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

3.3 Kurucz Databases

The Kurucz Atomic Line Lists were accessed via the Kurucz Atomic Database website (Kurucz 2024, 2011) and the data were scraped by 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 (Zhang et al. 2024)

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 dataset, 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, -16000, and -32000. 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 (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 dataset 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 dataset follows predefined 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 spectroscopic properties. The general JSON structure includes sections for Species, and Dataset (Dataset 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 Dataset Updates Each dataset 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 datasets, 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 dataset, allowing users to track updates efficiently. It begins with general information about the database, including the total count of atomic species, isotopes, and datasets 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 dataset sources and version numbers. This structure ensures that users can clearly distinguish between neutral atoms and their ionized states while maintaining consistency across datasets.

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, dataset source, and version number, see Appendix B.

Table 12 and Table 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 dataset 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_J, and state label QN (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 (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 (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 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

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
Dataset Information	
name	Dataset name
version	Dataset version (YYYYMMDD format)
doi	Digital Object Identifier for the dataset
max_temperature	Maximum temperature in dataset (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
Ionisation	Ionisation data (null if not available)
States Information	
number_of_states	Total number of states
max_energy	Maximum energy in dataset (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
Dataset Name	NIST, Kurucz
Version Number	20240601
Iron Ion (II)	
Atom Name	Iron Ion (II)
Chemical Formula	Fe_p
Number of Isotopes	1
Dataset Name	NIST, Kurucz
Version Number	20240601

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)
dataset	NIST
version	20240901

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. Firstly, 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 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 analyze 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. Table 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 labeled "CA", while measure empirical energies taken from NIST, are labeled "NI"; see 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 dataset 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 illustrates a representative sample (Li I) `.trans` file from 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 14. Specification of the ExoAtom `.states` file.

Field	Fortran format	C format	Description
ID	`I12`	`%12d`	State ID
$\tilde{E}$	`F12.6/`	`%12.6f/`	State energy in cm^{-1}
	`F12.5/F12.4`	`%12.5f/%12.4f`	
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}
$\tau^{\dagger}$	`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)

Note: 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:

- The ExoMol data standards use the given data formats for columns which should be separated by a single space.
- ID: Integer, starts from 1 and ends with the number of valid rows in levels data.
- $\tilde{E}$: 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`.
- g_J: Obtained directly from g in levels data. When the atom has isotopes, it corresponds to $g_{\rm tot}$; when the atom does not have isotopes, it corresponds to g_J.
- J: Obtained directly from J in levels data.
- Unc: Obtained directly from Uncertainty (cm^{-1}) in levels data.
- g: Obtained from Landé g-factor column in levels data. If this column is absent, it will not appear in the `.states` file.
- qn:configuration: Directly from the configuration column in levels data. The format should follow the `pyvalem` program (https://github.com/xnx/pyvalem).
- term: Directly from the term column in levels data. The trailing '*' should be removed if applicable. Format should be consistent with `pyvalem`.
- 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 +.
- 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	-

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

i	$\tilde{E}$	g_J	J	Unc	τ	gfactor	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

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

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

Field	Fortran format	C format	Description
i	`I12`	`%12d`	Upper state ID
f	`I12`	`%12d`	Lower state ID
A	`ES10.4`	`%10.4e`	Einstein A coefficient in s^{-1}
$\tilde{\nu}_{if}$	`E15.6`	`%15.6e`	Transition wavenumber in cm^{-1}

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:

- The ExoMol data standards use the given data formats for columns which should be separated by a single space.
- i: Determined by matching $\tilde{E}_k$, conf_k, J_k, and term_k in the lines data with $\tilde{E}$, Configuration, J, and Term in the levels data. The corresponding state ID in the levels data is assigned as the upper state ID. In cases where valid Term or J values are not provided in the lines data but are available in the levels data, matching is performed only using $\tilde{E}_k$ and conf_k.
- f: Determined by matching $\tilde{E}_i$, conf_i, J_i, and term_i in the lines data with $\tilde{E}$, Configuration, J, and Term in the levels data. The corresponding state ID in the levels data is assigned as the lower state ID. If valid Term or J values are absent in the lines data but exist in the levels data, matching is performed using only $\tilde{E}_i$ and conf_i.
- A: Directly obtained from A_{ki} (s^{-1}) in the lines data. Rows without a valid A_{ki} (s^{-1}) are removed.
- $\tilde{\nu}_{fi}$: Directly obtained from the wn (cm^{-1}) in the lines data.

Table 18. Extract from the transitions file for NIST database for Li I (neutral lithium atom), with columns formatted in ES15.6.

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

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 Alimohamadi & 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 (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 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. Figure 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% for Al, 0.1% for Mg, and 0.1% for Fe.

Table 21 and Table 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 dataset.

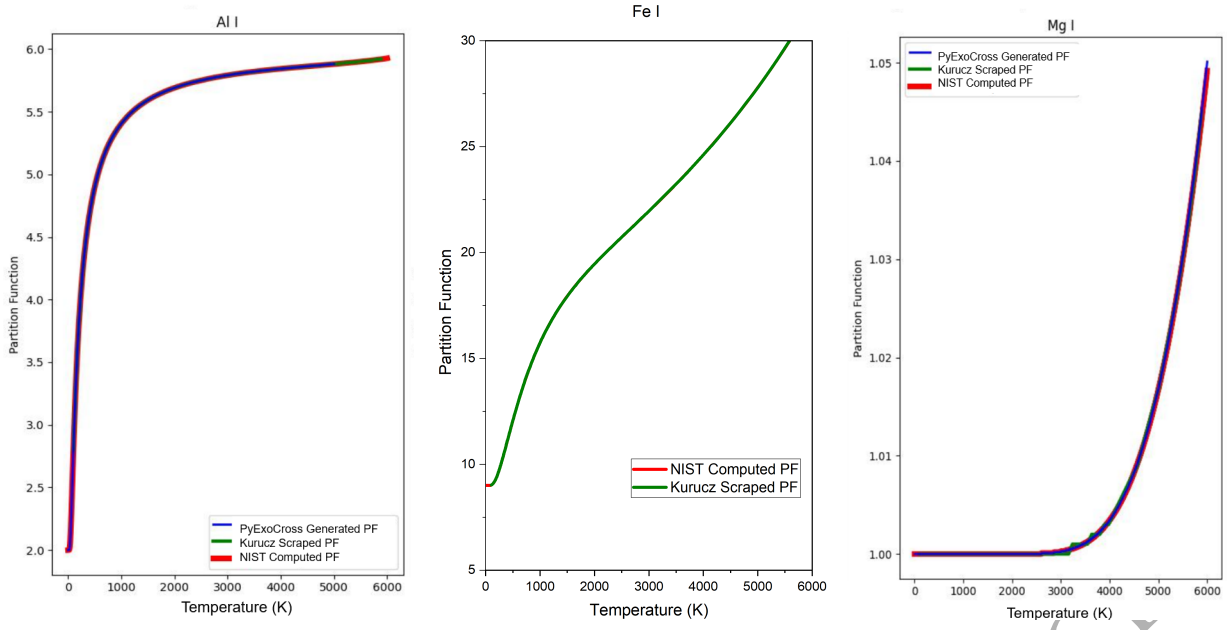

Figure 1. Comparison of partition functions for Al I, Fe I and Mg I, see text for further details.

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

- 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

4 POST PROCESSING

PyExoCross (Zhang et al. 2024) is a Python package that uses ExoMol-formatted 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.

The use of PyExoCross to generate spectra is illustrated in Figure 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

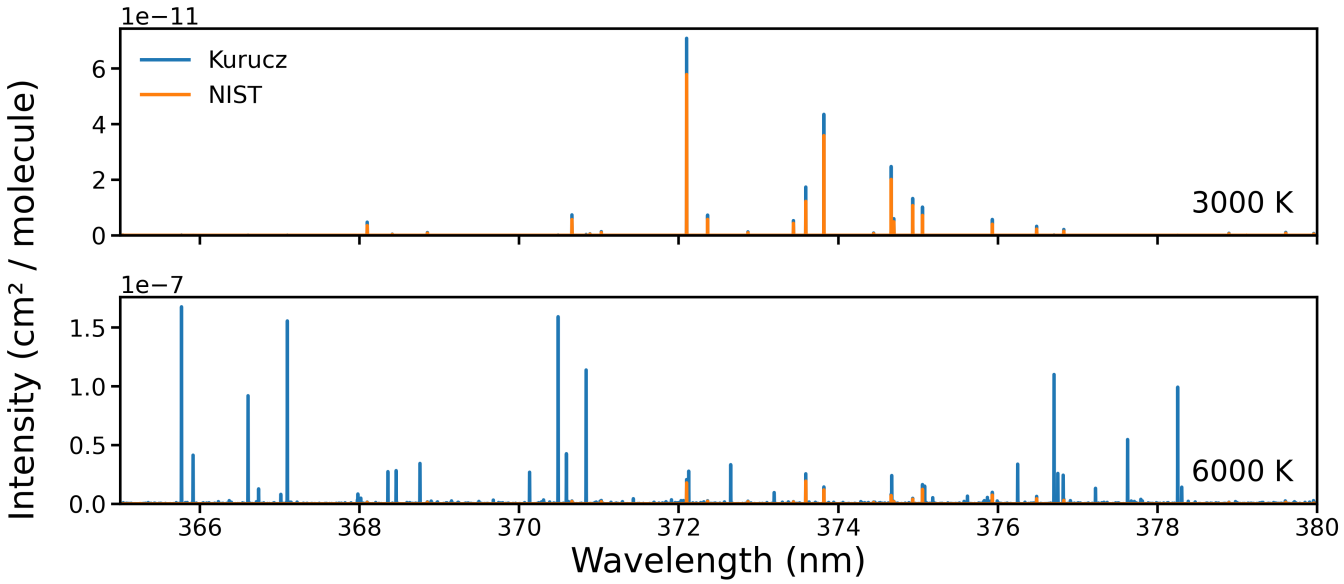

Figure 2. Comparison of NIST (Ralchenko & Kramida 2020) and Kurucz (Kurucz 2018) Fe I emission spectra at 3000 K and 6000 K; the 6000 K spectrum contains many lines only present in the Kurucz dataset.

differences for the predictied line intensities. For the NIST atomic database, uncertainties are provided for line positions (observed and Ritz wavelengths), but quantitative uncertainties for line intensities are generally not reported; however the NIST data for Fe I are substantially taken from Fuhr et al. (1988) who in turn use the highly accurate measured oscillator strengths of Blackwell et al. (1982). Conversely the Kurucz data appears to be taken from Peterson & Kurucz (2014) who computed oscillator strengths using the 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 datasets.

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 dataset. Thus, ExoAtom does not recommend one dataset over another but instead presents both to accommodate different research needs. These datasets play a crucial role in modeling atomic processes in astrophysical environments, including stellar atmospheres, exoplanetary spectra, and the interstellar medium. We note that while nearly all detections of atoms in exoplanets involve neutral or singly ionized species, some studies have focused on more highly ionized atoms (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 modeling and interpreting observations.

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Since we started this project, Robert (Bob) Kurucz passed away on 1 March 2025 (see Dupree & 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.

DATA AVAILABILITY

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

6 CONFLICT OF INTEREST

Authors declare no conflict of interest.

REFERENCES

Abjean, R. & Johannin-Gilles, A., 1975. Mesure des forces d'oscillateur par absorption dans un jet atomique—ii. force d'oscillateur de la transition $^1p_1 - ^1s_0$ du zn i (λ = 2139 å), *J. Quant. Spectrosc. Radiat. Transf.*, **15**, 25.

Alimohamadi, P. & Ferland, G. J., 2022. A Practical Guide to the Partition Function of Atoms and Ions, *PASP*, **134**.

Allard, N. F., Spiegelman, F., & Kielkopf, J. F., 2016. K–H_2 line shapes for the spectra of cool brown dwarfs, *A&A*, **589**, A21.

Allard, N. F., Spiegelman, F., Leininger, T., & Molliere, P., 2019. New study of the line profiles of sodium perturbed by H_2, *A&A*, **628**, A120.

Allehabi, S. O., Dzuba, V. A., & Flambaum, V. V., 2022. Atomic clocks highly sensitive to the variation of the fine-structure constant based on Hf II, Hf IV, and W VI ions, *Phys. Rev. A*, **106**, 032807.

Anderson, E. M., Zilitis, V. A., & Sorokina, E. S., 1967. Semiempirical calculation of oscillator strengths for Mg I, Ca I, and Sr I atoms, *Opt. Spectr.*, **23**, 102–105.

Anderson, T. & Sorensen, G., 1973. Atomic-state lifetimes of neutral and ionized Mg, Si, Cu and Zn, *J. Quant. Spectrosc. Radiat. Transf.*, **13**, 369–376.

Anisimove, G. P. & Semenov, R. I., 1974. Calculation of transition probabilities between the $3p^5ns$ configurations of Ne I and Ar I, *Opt. Spectr.*, **36**, 130.

Antena, A. A. & Zilitis, V. A., 1969. Semiempirical calculation of oscillator strengths for Zinc I, *Opt. Spectr.*, **26**, 79.

Artru, M. C., Jamar, C., Petrini, D., & Praderie, F., 1981. Autoionized levels and oscillator strengths for Si II, *A&A*, **90**, 380–39.

Badr, T., Plimmer, M. D., Juncar, P., Himbert, M. E., Louyer, Y., & Knight, D. J. E., 2006. Observation by two-photon laser spectroscopy of the $4d^{10}5s^2\ ^2S_{\frac{1}{2}} \rightarrow 4d^9 5s^2\ ^2D_{\frac{5}{2}}$ clock transition in atomic silver, *Phys. Rev. A*, **74**, 062509.

Banfield, F. P. & Huber, M. C. E., 1973. Oscillator strengths of Fe I transitions in the vacuum ultraviolet, *ApJ*, **186**, 335.

Baumann, S. R. & Smith, W. H., 1970. Atomic transition probabilities: Ultraviolet multiplet lifetimes of some Zn II, Cd II, and Hg II levels, *J. Opt. Soc. Am. B*, **60**, 345.

Bengston, R. D. & Miller, M. H., 1970. Experimental transition probabilities for neutral and ionized Ne, *J. Opt. Soc. Am.*, **60**, 1093.

Berry, H. G., Bromander, J., & Buchta, R., 1970a. Radiative lifetimes of excited levels in Li I, Mg I, Mg II, Al II, Al III, Si IV and K II, *Phys. Scr.*, **1**, 179–180.

Berry, H. G., Shectman, R. M., Martinson, I., Bickel, W. S., & Bashkin, S., 1970b. Beam-foil spectrum of Sulfur 1000-2000 A, *J. Opt. Soc. Am. B*, **60**, 335.

Berry, H. G., Bromander, J., Curtis, L. J., & Buchta, R., 1971. Lifetime measurements in Si II, Si III, Si IV and Al II, *Phys. Scr.*, **3**, 125.

Bielski, A., 1975. A critical survey of atomic transition probabilities for Cu I, *J. Quant. Spectrosc. Radiat. Transf.*, **15**, 463.

Biemont, E., 1973. Forces d'oscillateur pour des transitions de Mg I et Mg II, *Bull. Soc. Roy. Sci. Liege*, **42**, 206.

Biemont, E., Grevesse, N., Hannaford, P., & Lowe, R. M., 1981a. Oscillator strengths for Zr I and Zr II and a new determination of the solar abundance of zirconium, *ApJ*, **248**, 867–873.

Biemont, E., Grevesse, N., Kwiatkovski, M., & Zimmermann, P., 1981b. Radiative lifetimes in Ru I, *A&A*, **131**, 364–366.

Biemont, E., Grevesse, N., Kwiatkovski, M., & Zimmermann, P., 1981c. Radiative lifetimes in Ti I and Ti II, *A&A*, **108**, 127–229.

Black, J. H., Wisheit, J. C., & Laviana, E., 1972. Oscillator strengths and ground-state photoionization cross-sections for Mg II and Ca II, *ApJ*, **177**, 567.

Blackwell, D. E. & Collins, B. S., 1972. Oscillator strengths for excitation of Helium and Helium-like ions by electron impact, *MNRAS*, **157**, 255.

Blackwell, D. E., Ibbetson, P. A., Petford, A. D., & Shallis, M. J., 1979. Precision measurements of relative oscillator strengths—IV. Fe I transitions, *MNRAS*, **186**, 633.

Blackwell, D. E., Petford, A. D., Shallis, M. J., & Simmons, G. J., 1982. Precision-Measurement Of Relative Oscillator-Strengths .9. Measures Of Fe-I Transitions From Levels A5P1-3(2.18-2.28eV), A3P2(2.28eV), A3P0,1(2.49-2.42eV), Z7(D0(1-5)(2.48-2.40eV) And A3H4-6(2.45-2.40eV), *MNRAS*, **199**, 43–51.

Blaise, J., J. Vergès, Wyart, J.-F., & Engleman Jr., R., 1992. Energy levels of neutral platinum (Pt I), *J. Phys. II France*, **2**, 947–957.

Bridges, J. M. & Kornblith, R. L., 1974. ARC measurements of Fe I oscillator strengths, *ApJ*, **192**, 793.

Bridges, J. M. & Wiese, W. L., 1967. Experimental determination of transition probabilities for S I and S II, *Phys. Rev.*, **159**, 31.

Bromander, J., 1971. Lifetimes of excited levels in B I, B II, C II, Mg I and Mg II, *Phys. Scr.*, **4**, 61.

Bromander, J.and Duric, N., Erman, P., & Larsson, M., 1978. Lifetimes of excited levels in Mg I, Mg II, Mg III, C I and Si II, *Phys. Scr.*, **17**, 119.

Brooks, N. H., Rohrlich, D., & Smith, W. H., 1977. Transition probabilities in neutral Carbon and Nitrogen, *ApJ*, **214**, 328.

Brown, C. M., Tilford, S. G., & Ginter, M. L., 1977. Absorption spectrum of Sn I between 1580 and 2040 Å, *J. Opt. Soc. Am.*, **67**, 607–621.

Byard, P. L., 1968. Absolute transition probabilities for lines of Cr I and Cr II, *J. Quant. Spectrosc. Radiat. Transf.*, **8**, 1543.

Callender, C. L., Hackett, P. A., & Rayner, D. M., 1988. First-ionization potential of ruthenium, rhodium, and palladium by double-resonance ionization spectroscopy, *J. Opt. Soc. Am. B*, **5**, 614–618.

Cardon, B. L., Parkinson, W. H., & Tomkins, F. S., 1980. Oscillator strengths of Y I and Y II transitions, *J. Opt. Soc. Am.*, **70**, 1372.

Castelli, F. & Kurucz, R. L., 2010. New Fe II energy levels from stellar spectra, *A&A*, **520**, A57.

Castelli, F., Kurucz, R. L., & Cowley, C. R., 2015. New Mn II energy levels from the STIS-HST spectrum of the HgMn star HD 175640, *A&A*, **580**, A10.

Caves, T. C., 1975. Electric quadrupole transitions in Li I, *J. Quant. Spectrosc. Radiat. Transf.*, **15**, 439.

Cerny, D., Bacis, R., Bussery, B., Nota, M., & Vergès, J., 1991. Experimental determination and calculation of the collision relaxation rates in the 5 $^2P_{\frac{1}{2}}$ and 5 $^2P_{\frac{3}{2}}$ levels of atomic iodine, *The Journal of Chemical Physics*, **95**, 5790–5798.

Cheng, K. T. & Johnson, W. R., 1977. Excitation energies and f-values in the B isoelectronic sequence, *Phys. Rev. A*, **15**, 1326–1329.

Chubb, K. L., Rocchetto, M., Yurchenko, S. N., Min, M., Waldmann, I., Barstow, J. K., Molliere, P., Al-Refaie, A. F., Phillips, M., & Tennyson, J., 2021. The ExoMolOP Database: Cross-sections and k-tables for Molecules of Interest in High-Temperature Exoplanet Atmospheres, *A&A*, **646**, A21.

Cock, C. L., Stark, A., & Evans, J. C., 1973. Absolute oscillator strengths in Cr I, *ApJ*, **184**, 653.

Cohen, M. & McEachran, R. P., 1978. The Hartree-Fock approximation for S-states of Carbon, *J. Quant. Spectrosc. Radiat. Transf.*, **20**, 295.

Cook, E. C., Vira, A. D., & Williams, W. D., 2020. Resonant two-photon spectroscopy of the $2s3d\ ^1D_2$ level of neutral ^{9}Be, *Phys. Rev. A*, **101**, 042503.
Corliss, C. H., 1970. Relative probabilities for transitions in the Cu I spectrum, *J. Res. Nat. Bur. Stand.*, **74A**, 781.
Corliss, C. H. & Bozman, W. R., 1962. Experimental transition probabilities for spectral lines of seventy elements, NBS Monograph 53.
Cowan, R. D., 1981. *The Theory of Atomic Structure and Spectra*, Los Alamos Series in Basic and Applied Sciences, Univ. of California Press, Berkeley, CA.
Cowan, R. D., Hobbs, L. M., & York, D. G., 1982. Oscillator strengths for resonance transitions of neutral Carbon, *ApJ*, **257**, 373–375.
Cowley, C. R. & Corliss, C. H., 1983. A comparison of Corliss-Bozman oscillator strengths with improved values, *MNRAS*, **203**, 651–659.
Curry, J. J., 2004. Compilation of Wavelengths, Energy Levels, and Transition Probabilities for Ba I and Ba II, *J. Phys. Chem. Ref. Data*, **33**, 725–746.
Curtis, L. J. & Smith, W. H., 1974. Radiative-lifetime measurements of levels in Si II, Si III, Si IV, and C II, *Phys. Rev. A*, **9**, 1537.
Dammalapati, U., Jungmann, K., & Willmann, L., 2016. Compilation of Spectroscopic Data of Radium (Ra I and Ra II), *J. Phys. Chem. Ref. Data*, **45**, 013101.
D'Arpa, M. C., Saba, A., Borsa, F., Fossati, L., Micela, G., Di Maio, C., Stangret, M., Tripodo, G., Affer, L., Bonomo, A. S., Benatti, S., Brogi, M., Fardella, V., Lanza, A. F., Guilluy, G., Maldonado, J., Mantovan, G., Nascimbeni, V., Pino, L., Scandariato, G., Sicilia, D., Sozzetti, A., Spinelli, R., Andreuzzi, G., Bignamini, A., Claudi, R., Desidera, S., Ghedina, A., Knapic, C., & Lorenzi, V., 2024. "The GAPS programme at TNG: LX. Atmospheric characterisation of KELT-9 b via single-line analysis: Detection of six H I Balmer lines, Na I, Ca I, Ca II, Fe I, Fe II, Mg I, Ti II, Sc II, and Cr II", *A&A*, **690**, A237.
Del Zanna, G., Dere, K. P., Young, P. R., & Landi, E., 2021. CHIANTI—An Atomic Database for Emission Lines. XVI. Version 10, Further Extensions, *ApJ*, **909**, 38.
Demirdak, G., Sahin, E., & Ertürk, M., 2023. Generalized complete orthonormal sets of Exponential-Type functions, *Chemical Physics*, **570**, 111893.
Den Hartog, E. A., Lawler, J. E., Sneden, C., & Cowan, J. J., 2003. Improved laboratory transition probabilities for Nd II and application to the neodymium abundances of the sun and three metal-poor stars, *ApJS*, **148**, 543–566.
Den Hartog, E. A., Herd, M. T., Lawler, J. E., Sneden, C., Cowan, J. J., & Beers, T. C., 2005. Improved laboratory transition probabilities for Pt I and application to the platinum abundances of BD + 17°3248 and the Sun, *ApJ*, **619**, 639–655.
Den Hartog, E. A., Palmer, A. J., & Lawler, J. E., 2015. Radiative lifetimes and transition probabilities of neutral lanthanum, *J. Phys. B-At. Mol. Opt. Phys.*, **48**, 155001.
Desai, S. V. & Corcoran, W. H., 1968. Numerical transition probabilities for Ar I, *J. Quant. Spectrosc. Radiat. Transf.*, **8**, 1721.
Dolk, L., Litzén, U., & Wahlgren, G. M., 2002. The laboratory analysis of Bi III and its application to the Bi-rich HgMn star HR 7775, *A&A*, **388**, 692–703.
Drake, G. W., 1988. Theoretical energies for the $n = 1$ and 2 states of the helium isoelectronic sequence up to $Z = 100$, *Can. J. Phys.*, **66**, 586–611.
Druetta, M., Poulizac, M. C., & Desequelles, J., 1970. Mean-life measurements in C II, C III, and C IV, *J. Opt. Soc. Am.*, **60**, 1463.
Dumont, P. D., Biemont, E., & Grevesse, N., 1974. Transition probabilities for transitions of the nitrogen isoelectronic sequence, *J. Quant. Spectrosc. Radiat. Transf.*, **14**, 1127.
Dupree, A. & Conroy, C., 2025. Robert Kurucz (1944–2025), *Nature Astronomy*.
Duquette, D. W. & Lawler, J. E., 1982. Radiative lifetimes of upper levels in Nb I, *Phys. Rev. A*, **26**, 330–334.
Duquette, D. W. & Lawler, J. E., 1985. Radiative lifetimes of the z 2D states in Mo I, *J. Opt. Soc. Am. B*, **2**, 1948.
Duquette, D. W., Den Hartog, E. A., & Lawler, J. E., 1986. Absolute transition probabilities in Nb I and Hf I and a solution to the problem of missing infrared branches, *J. Quant. Spectrosc. Radiat. Transf.*, **35**, 281–301.
Engleman, R., Litzén, U., Lundberg, H., & Wyart, J.-F., 1998. The Pd I Spectrum, Term System, Isotope Shift and Hyperfine Structure – Revised and Extended Analysis Based on FTS Emission Spectroscopy, *Phys. Scr.*, **57**, 345.
Fedchak, J. A., Den Hartog, E. A., Lawler, J. E., Palmeri, P., Quinet, P., & Biémont, E., 2000. Experimental and theoretical radiative lifetimes, branching fractions, and oscillator strengths for Lu I and experimental lifetimes for Lu II and Lu III, *ApJ*, **542**, 1109–1118.
Figger, H., Heldt, J., Siomos, K., & Walther, H., 1975. Radiative lifetimes of highly excited states in Fe I, *A&A*, **43**, 389.
Fivet, V., Palmeri, P., Quinet, P., Biémont, E., Xu, H. L., & Svanberg, S., 2006a. Radiative lifetimes and transition probabilities in Ta I, *Eur. Phys. J. D*, **37**, 29–35.
Fivet, V., Quinet, P., Biémont, E., & Xu, H. L., 2006b. Transition probabilities and lifetimes in gold (Au I and Au II), *J. Phys. B-At. Mol. Opt. Phys.*, **39**, 3587–3598.
Fossati, L., Haswell, C. A., Froning, C. S., Hebb, L., Holmes, S., Kolb, U., Helling, C., Carter, A., Wheatley, P., Cameron, A. C., Loeillet, B., Pollacco, D., Street, R., Stempels, H. C., Simpson, E., Udry, S., Joshi, Y. C., West, R. G., Skillen, I., & Wilson, D., 2010. Metals in the exosphere of the highly irradiated planet WASP-12b, *ApJL*, **714**, L222–L227.
Foster, E. W., 1967. Measurement of transition probabilities in the CI multiplet 2p2 3P-2p3s 3P0, *Proc. Phys. Soc.*, **90**, 275.
Friedrich, H. & Trefftz, E., 1970. Configuration interaction and oscillator strengths for Nitrogen ions, MPI-PAE/Astro preprint.
Froese Fischer, C., 1975a. Theoretical oscillator strengths for nS-mP transitions in Mg I, *Can. J. Phys.*, **53**, 184.
Froese Fischer, C., 1975b. Theoretical oscillator strengths for the 3s2 1S - 3s 3p 1P transition in Mg I, *J. Opt. Soc. Am.*, **69**, 118.
Fuhr, J. R. & Wiese, W. L., 1996. NIST atomic transition probability tables, in *CRC Handbook of Chemistry and Physics*, chap. 10, eds Lide, D. R. & Frederikse, H. P. R., CRC Press, Boca Raton, FL, 77th edn.
Fuhr, J. R. & Wiese, W. L., 2005. NIST Atomic Transition Probabilities, in *CRC Handbook of Chemistry and Physics*, ed. Lide, D. R., CRC Press, Boca Raton, FL, 86th edn.
Fuhr, J. R. & Wiese, W. L., 2006. A critical compilation of atomic transition probabilities for neutral and singly ionized iron, *J. Phys. Chem. Ref. Data*, **35**, 1669–1809.
Fuhr, J. R. & Wiese, W. L., 2010. Tables of atomic transition probabilities for beryllium and boron, *J. Phys. Chem. Ref. Data*, **39**, 013101.
Fuhr, J. R., Martin, G. A., Wiese, W. L., & Younger, S. M., 1981. Atomic transition probabilities for Iron, Cobalt, and Nickel, *J. Phys. Chem. Ref. Data*, **10**, 305.
Fuhr, J. R., Martin, G. A., & Wiese, W. L., 1988. Atomic Transition Probabilities–Iron through Nickel, *J. Phys. Chem. Ref. Data*, **17**, 1–493.
Gamache, R. R., Vispoel, B., Tennyson, J., Yurchenko, S. N., Polyansky, O. L., Gordon, I. E., Hargreaves, R. J., & Huang, X., 2025. Partition sums for molecules and their isotopologues on HITRAN2024, *J. Quant. Spectrosc. Radiat. Transf.*, **345**, 109568.
Garstang, R. H. & Odabasi, H., 1971. *Topics in Modern Physics*, pp. 361–286, Colorado Associated University Press, Boulder, Colarodo, US.
Garz, T., 1973. Relative oscillator strengths for Si I, *A&A*, **26**, 471.
Gil, G. & Gonzalez, A., 2017. The NIST compilation of ionization potentials revisited (I): From He-like to Xe-like ions, *Can. J. Phys.*, **95**, 479–497.
Goly, A., 1976. Experimental oscillator strengths for some transitions of C I, *A&A*, **52**, 43.
Goly, A., Moity, J., & Weniger, S., 1975. Experimental oscillator strengths for Ni II lines, *A&A*, **38**, 259.
Grasdalen, G. L., Huber, M., & Parkinson, W. H., 1969. Absolute gf-values for Fe I and Fe II lines, *ApJ*, **156**, 1153.
Greenlee, T. R. & Whaling, W., 1979. Absolute transition probabilities in Mn I, *J. Quant. Spectrosc. Radiat. Transf.*, **21**, 55.
Grevess, N. & Swings, J. P., 1972. Oscillator strengths for Si I and solar abundance of Silicon, *ApJ*, **171**, 179.

Güzelçimen, F., Tonka, M., Uddin, Z., Bhatti, N. A., Windholz, L., Kröger, S., & Başar, G., 2018. Revised energy levels of singly ionized lanthanum, *J. Quant. Spectrosc. Radiat. Transf.*, **211**, 188–199.

Hannaford, P., Lowe, R. M., Grevesse, N., Biémont, E., & Whaling, W., 1982. Oscillator strengths for Y I and Y II and the solar abundance of yttrium, *ApJ*, **261**, 736–746.

Hannaford, P., Lowe, R. M., Biemont, E., & Grevesse, N., 1985. Oscillator strengths in the B isoelectronic sequence, *A&A*, **143**, 447–450.

Haris, K. & Kramida, A., 2017. Critically evaluated spectral data for neutral carbon (C I), *ApJS*, **233**, 16.

Haris, K., Kramida, A., & Tauheed, A., 2014. Extended and revised analysis of singly ionized tin: Sn II, *Phys. Scr.*, **89**, 115403.

Hassini, F., Ahmed, Z. B., Robaux, O., Vergès, J., & Wyart, J.-F., 1988. Study of fine and hyperfine structures in the spectrum of neutral antimony (^{121}Sb I), *J. Opt. Soc. Am. B*, **5**, 2060–2075.

Heise, H., 1974. Experimental oscillator strengths for Ni I and Ni II lines, *A&A*, **34**, 275.

Hibbert, A., 1974. Radiative lifetimes and oscillator strengths for Nb II, *J. Phys.B-At. Mol. Phys.*, **7**, 1417.

Hibbert, A., 1988. Oscillator strengths for transitions in P II, *Phys. Scr.*, **38**, 37–44.

Hilborn, R. C. & de Zafra, R., 1973. Experimental absolute oscillator strengths for transitions in Fe I, *ApJ*, **183**, 347.

Hoeijmakers, H. J., Ehrenreich, D., Kitzmann, D., Allard, R., Grimm, S. L., Seidel, V, J., Wyttenbach, A., Pino, L., Nielsen, L. D., Fisher, C., Rimmer, P. B., Bourrier, V., Cegla, H. M., Lavie, B., Lovis, C., Patzer, A. B. C., Stock, J. W., Pepe, F. A., & Heng, K., 2019. A spectral survey of an ultra-hot Jupiter Detection of metals in the transmission spectrum of KELT-9 b, *A&A*, **627**, A165.

Hoeijmakers, H. J., Seidel, V, J., Pino, L., Kitzmann, D., Sindel, J. P., Ehrenreich, D., Oza, V, A., Bourrier, V., Allart, R., Gebek, A., Lovis, C., Yurchenko, S. N., Astudillo-Defru, N., Bayliss, D., Cegla, H., Lavie, B., Lendl, M., Melo, C., Murgas, F., Nascimbeni, V., Pepe, F., Segransan, D., Udry, S., Wyttenbach, A., & Heng, K., 2020. Hot Exoplanet Atmospheres Resolved with Transit Spectroscopy (HEARTS): IV. A spectral inventory of atoms and molecules in the high-resolution transmission spectrum of WASP-121 b, *A&A*, **641**, A123.

Hoeijmakers, H. J., Kitzmann, D., Morris, B. M., Prinoth, B., Borsato, N. W., Thorsbro, B., Pino, L., Lee, E. K. H., Akin, C., Seidel, J. V., Birkby, J. L., Allart, R., & Heng, K., 2024. The Mantis Network IV. A titanium cold trap on the ultra-hot Jupiter WASP-121 b, *A&A*, **685**, A139.

Holovaty, A., Willison, S., et al., 2003. Django web framework, *URL http://www. djangoproject. com*.

Huber, M. C. E., 1974. Interferometric gas-flow measurements of Fe I oscillator strengths, *ApJ*, **190**, 237.

Huber, M. C. E. & Sandeman, R. J., 1977. Oscillator strengths of Cr I lines lying between 200 and 541 nm, *Proc. R. Soc. London, Ser. A*, **357**, 355.

Huber, M. C. E. & Tobey, F. L., 1968. gf-values of Fe I lines in the range 2550-2800 A, *ApJ*, **152**, 609.

Huber, M. C. E., Sandeman, R. J., & Tubbs, E. F., 1975. The absorption spectrum of Cr I between 1750 and 2050 A, *Proc. R. Soc. London, Ser. A*, **342**, 431.

Humphreys, C. J., Paul, E., & Minnhagen, L., 1971. First Spectra of Chlorine, Bromine, and Iodine in the 4-μm Region, *J. Opt. Soc. Am.*, **61**, 110–114.

Jiang, Z., Wang, W., Zhao, G., Zhai, M., Shi, Y., Liu, Y., Zhao, J., & Chen, Y., 2023. Detection of Rubidium and Samarium in the Atmosphere of the Ultrahot Jupiter MASCARA-4b, *AJ.*, **165**, 230.

Jitrik, O. & Bunge, C. F., 2005. Transition Probabilities for Hydrogen-Like Atoms, *J. Phys. Chem. Ref. Data*, **33**, 1059–1070.

Kahl, E. V., Berengut, J. C., Laatiaoui, M., Eliav, E., & Borschevsky, A., 2019. High-precision ab initio calculations of the spectrum of Lr^+, *Phys. Rev. A*, **100**, 062505.

Kandula, D. Z., Gohle, C., Pinkert, T. J., Ubachs, W., & Eikema, K. S. E., 2010. Extreme Ultraviolet Frequency Comb Metrology, *Phys. Rev. Lett.*, **105**, 063001.

Karlsson, H. & Litzén, U., 2001. Hyperfine constants, revised wavelengths and energy levels in In I and In II derived by Fourier transform spectroscopy, *Journal of Physics B: Atomic, Molecular and Optical Physics*, **34**, 4475.

Karlsson, H., Joueizadeh, A., & Johansson, S., 2002. Ru II Wavelengths and Energy Levels Derived by Fourier Transform Spectroscopy, *Phys. Scr.*, **66**, 238.

Kelleher, D. E. & Podobedova, L. I., 2008a. Atomic transition probabilities of sodium and magnesium. A critical compilation, *J. Phys. Chem. Ref. Data*, **37**, 267–706.

Kelleher, D. E. & Podobedova, L. I., 2008b. Atomic transition probabilities of aluminum. A critical compilation, *J. Phys. Chem. Ref. Data*, **37**, 709–911.

Kelleher, D. E. & Podobedova, L. I., 2008c. Atomic transition probabilities of silicon. A critical compilation, *J. Phys. Chem. Ref. Data*, **37**, 1285–1501.

Kelly, R. L., 1987. Atomic and ionic spectrum lines below 2000 Angstroms. Hydrogen through Krypton, *J. Phys. Chem. Ref. Data*, **17**.

King, R. B., 1947a. Relative gf-values for lines of V I, *ApJ*, **105**, 376.

King, R. B., 1947b. Relative gf-values for lines of Ni I, *ApJ*, **108**, 87.

Klemt, M., 1973. Experimentelle Oszillatorenstärken von Ti I-Linien, *A&A*, **29**, 419.

Kock, M. & Richter, J., 1968. Experimentelle Übergangswahrscheinlichkeiten und solare Häufigkeit des Kupfers, *Z. Astrophys.*, **69**, 180.

Kramida, A., 2013a. Critically evaluated energy levels and spectral lines of singly ionized indium (In II), *J. Res. Natl. Inst. Stand. Technol.*, **118**, 52–104.

Kramida, A., 2013b. A critical compilation of energy levels, spectral lines, and transition probabilities of singly ionized silver, Ag II, *J. Res. Natl. Inst. Stand. Technol.*, **118**, 168–198.

Kramida, A., 2022. Update of atomic data for the first three spectra of actinium, *Atoms*, **10**, 42.

Kramida, A. & Haris, K., 2022. Critically evaluated spectral data for singly ionized carbon (C II), *ApJS*, **260**, 11.

Kramida, A. & Nave, G., 2008. The Ne II Spectrum, *Eur. Phys. J. D*, **39**, 331–350.

Kramida, A. & Sansonetti, J. E., 2013. Energy levels and spectral lines of singly ionized manganese (Mn II), *ApJS*, **205**, 14.

Kramida, A., Yu. Ralchenko, Reader, J., & and NIST ASD Team, 2015. NIST Atomic Spectra Database (ver. 5.3), [Online]. Available: `http://physics.nist.gov/asd` [2017, April 2]. National Institute of Standards and Technology, Gaithersburg, MD.

Kramida, A., Nave, G., & Reader, J., 2017. The Cu II spectrum, *Atoms*, **5**, 9.

Kramida, A. E., 2005. Critical Compilation of Wavelengths and Energy Levels of Singly Ionized Beryllium (Be II), *Phys. Scr.*, **72**, 309.

Kramida, A. E., 2010. A critical compilation of experimental data on spectral lines and energy levels of hydrogen, deuterium, and tritium, *Atomic Data and Nuclear Data Tables*, **96**, 586–644.

Kramida, A. E. & Ryabtsev, A. N., 2007. A critical compilation of energy levels and spectral lines of neutral boron, *Phys. Scr.*, **76**, 544.

Kramida, A. E. & Shirai, T., 2006. Compilation of wavelengths, energy levels, and transition probabilities for W I and W II, *J. Phys. Chem. Ref. Data*, **35**, 423–683.

Kurucz, R. L., 1975. unpublished.

Kurucz, R. L., 1988. *Semiempirical gf-values for Fe II*, chap. XXB, pp. 168–172, Kluwer, Dordrecht, Netherlands.

Kurucz, R. L., 2002. Atomic and Molecular Data Needs for Astrophysics, *AIP Conference Proceedings*, **636**, 134–143.

Kurucz, R. L., 2011. Including all the lines, *Can. J. Phys.*, **89**, 417–428.

Kurucz, R. L., 2014. *Problems with Atomic and Molecular Data: Including All the Lines*, pp. 63–73, Springer International Publishing, Cham.

Kurucz, R. L., 2018. Including All the Lines: Data Releases for Spectra and Opacities through 2017, in *WORKSHOP ON ASTROPHYSICAL OPACITIES*, vol.

515 of **ASP**, pp. 47–54, Western Michigan Univ, Coll Arts & Sci; Western Michigan Univ, Dept Phys, Workshop on Astrophysical Opacities, Western Michigan Univ, Foster Ctr, Kalamazoo, MI, AUG 01-04, 2017.

Kurucz, R. L., 2024. Kurucz/Atoms, http://kurucz.harvard.edu/atoms.html, Accessed: 01-June-2024.

Kurucz, R. L. & Peytremann, E., 1975. A table of semiempirical gf-values, SAO Special Report 362.

Kurucz, R. L., Hubeny, I., Stone, J. M., MacGregor, K., & Werner, K., 2009. Including All the Lines, in *AIP Conference Proceedings*, AIP.

Kwiatkowski, M., Zimmermann, P., Biemont, E., & Grevesse, N., 1982. Radiative lifetimes in Rh I, *A&A*, **112**, 337–340.

Lambert, D., 1968. The abundance of the elements in the solar photosphere—I. Carbon, Nitrogen and Oxygen, *MNRAS*, **138**, 143.

Lambert, D. L., Mallia, E. A., & Warner, B., 1969. The abundance of the elements in the solar photosphere—X. Magnesium, *MNRAS*, **142**, 71.

Laughlin, C., 1978. The 2s2 1S0-2s2p 3P1 intercombination transition in Be I, *J. Phys.B-At. Mol. Phys.*, **11**, L391.

Laughlin, C. & Dalgarno, A., 1973. Nuclear charge expansion method for 1snl 1,3L-1sn'l' 1,3L' transitions in the Helium sequence, *Phys. Rev. A*, **8**, 39.

Laughlin, C. & Victor, G. A., 1974. Multiplet splittings and 1S0-3P1 intercombination-line oscillator strengths in Be I and Mg I, *ApJ*, **192**, 551.

Laughlin, C., Constantinides, E. R., , & Victor, G. A., 1978. Two-photon absorption and transition probabilities in the B isoelectronic sequence, *J. Phys.B-At. Mol. Phys.*, **11**, 2243.

Laurent, J. & Weniger, S., 1970. Etude des probabilites de transition de quelques raies de Ni I et Ni II, *J. Quant. Spectrosc. Radiat. Transf.*, **10**, 315.

Lawler, J. E., Bonvallet, G., & Sneden, C., 2001. Experimental radiative lifetimes, branching fractions, and oscillator strengths for La II and a new determination of the solar lanthanum abundance, *ApJ*, **556**, 452–460.

Lawler, J. E., Sneden, C., Cowan, J. J., Ivans, I. I., & Den Hartog, E. A., 2009. Improved laboratory transition probabilities for Ce II, application to the cerium abundances of the sun and five r-process-rich, metal-poor stars, and rare earth lab data summary, *ApJS*, **182**, 51–79.

Lawler, J. E., Chisholm, J., Nitz, D. E., Wood, M. P., Sobeck, J., & Den Hartog, E. A., 2010. Atomic transition probabilities of Ce I from Fourier transform spectra, *J. Phys. B-At. Mol. Opt. Phys.*, **43**, 085701.

Lawler, J. E., Schmidt, J. R., & Den Hartog, E. A., 2022. Energy Levels of Singly Ionized and Neutral Hafnium, *ApJS*, **258**, 27.

Lawrence, G. M., 1967. Resonance transition probabilities in intermediate coupling for Cu II, Ag II, and Au II, *ApJ*, **148**, 261.

Lennard, W. N., Whaling, W., Scalo, J. M., & Testerman, L., 1975. Ni I transition probabilities and the solar Nickel abundance, *ApJ*, **197**, 517.

Li, R., Chatelain, R., Holt, R. A., Rehse, S. J., Rosner, S. D., & Scholl, T. J., 2007. Oscillator strength measurements in Pr II with the fast-ion-beam laser-induced-fluorescence technique, *Phys. Scr.*, **76**, 577–592.

Lilly, R. A., 1975. Transition probabilities in the spectra of Ne I, *J. Opt. Soc. Am.*, **65**, 389.

Lilly, R. A., 1976. Transition probabilities in the spectra of Ne I, *J. Opt. Soc. Am.*, **66**, 245.

Lincke, R. & Ziegenbein, G., 1971. Messung der Übergangswahrscheinlichkeiten von Linien des Mg I, Mg II, Ca I, Ca II und Sr I, *Z. Phyzik*, **241**, 369.

Lindgard, A. & Nielsen, S. E., 1977. Transition probabilities for the Alkali isoelectronic sequences, *At. Data Nucl. Data Tables*, **19**, 533.

Linsky, J. L., Yang, H., France, K., Froning, C. S., Green, J. C., Stocke, J. T., & Osterman, S. N., 2010. Observations of mass loss from the transiting exoplanet HD 209458b, *ApJ*, **717**, 1291–1299.

Litzén, U., Brault, J. W., & Thorne, A. P., 1993. Spectrum and term system of neutral nickel, Ni I, *Phys. Scr.*, **47**.

Livingston, A. E., Kernahan, J. A., Irwin, D. J. G., & Pinnington, E. H., 1975. Beam-foil studies of Phosphorus in the vacuum ultraviolet, *Phys. Scr.*, **12**, 223–229.

Loginov, A. V. & Gruzdev, P. F., 1978a. Probabilities of 2p5np-2p5ms (m=3, 4) transitions in the spectrum of Ne I, *Opt. Spectr.*, **44**, 123.

Loginov, A. V. & Gruzdev, P. F., 1978b. Probabilities of 3p5np-3p5ms transitions in the spectrum of Ar I, *Opt. Spectr.*, **44**, 500–503.

Lombardi, G. G., Cardon, B. L., & Kurucz, R. L., 1981. Oscillator strengths of neutral aluminum lines in the vacuum ultraviolet, *ApJ*, **248**, 1202–1208.

Lotrian, J., Cariou, J., & Johannin-Gilles, A., 1975. Determination of transition probabilities of Ti II lines, *J. Quant. Spectrosc. Radiat. Transf.*, **15**, 815.

Lundberg, H., Tchang-Brillet, W.-U. L., Launay, F., & Engleman, R., 2001. Analysis of the Pd II Spectrum in the Ultraviolet and Infrared Regions, *Phys. Scr.*, **64**, 63.

Luyken, B. F. W., 1972. Transition probabilities and radiative lifetimes in Ar II, *Physica*, **60**, 432.

Makdisi, Y. & Bhatia, K. S., 1982. Ultraviolet and visible spectra of tellurium I, *J. Phys.B-At. Mol. Phys.*, **15**, 909.

Martin, G. A., Fuhr, J. R., & Wiese, W. L., 1988. Atomic Transition Probabilities–Scandium through Manganese, *J. Phys. Chem. Ref. Data*, **17**, 512.

Martin, P. & Campos, J., 1977. Experimental transition probabilities of some Ne I lines, *J. Opt. Soc. Am.*, **67**, 1327.

Martin, P. & Campos, J., 1978. Lifetimes of some excited states of Ne I, *J. Quant. Spectrosc. Radiat. Transf.*, **19**, 109.

Martin, P. & Campos, J., 1979. Transition probabilities of lines of Ne I and Ne II, *J. Quant. Spectrosc. Radiat. Transf.*, **22**, 183.

Martin, W. C. & Zalubas, R., 1979. Energy levels of aluminum, Al I through Al XIII, *J. Phys. Chem. Ref. Data*, **8**, 817–864.

Martin, W. C. & Zalubas, R., 1980. Energy levels of magnesium, Mg I through Mg XII, *J. Phys. Chem. Ref. Data*, **9**, 1–58.

Martin, W. C. & Zalubas, R., 1983. Energy Levels of Silicon, Si I through Si XIV, *J. Phys. Chem. Ref. Data*, **12**, 323–380.

Martin, W. C., Zalubas, R., & Musgrove, A., 1985. Energy Levels of Phosphorus, P I through P XV, *J. Phys. Chem. Ref. Data*, **14**, 751–802.

Martin, W. C., Zalubas, R., & Musgrove, A., 1990. Energy Levels of Sulfur, S I Through S XVI, *J. Phys. Chem. Ref. Data*, **19**, 821–880.

Martin, W. C., Wiese, W. L., & Kramida, A., 2023. *Atomic Spectroscopy*, pp. 177–197, Springer International Publishing, Cham.

Martinson, I., Bickel, W., & Olme, A., 1970. Beam-foil excitation and lifetimes of levels in B I, B II and B III, *J. Opt. Soc. Am.*, **60**, 1213.

May, M., Richter, J., & Wichelmann, J., 1974. Experimental oscillator strengths of weak Fe I lines, *A&AS*, **18**, 405.

Mazing, M. A. & Serapinas, P. D., 1969. Oscillator strengths of high n lines of Rb I and Cs I, *Opt. Spectr.*, **27**, 482–485.

McEachran, R. P. & Cohen, M., 1971. Theoretical oscillator strengths for the Boron isoelectronic sequence, *J. Quant. Spectrosc. Radiat. Transf.*, **11**, 1819.

McKemmish, L. K., Bowesman, C. A., Kefala, K., Perri, A. N., Syme, A. M., Yurchenko, S. N., & Tennyson, J., 2024. A hybrid approach to generating diatomic line lists for high resolution studies of exoplanets and other hot astronomical objects: Updates to ExoMol MgO, VO and TiO line lists, *RASTI*, **3**, 565–583.

Meggers, W. F., Corliss, C. H., & Scribner, B. F., 1975. Tables of Spectral-Line Intensities, NBS Monograph 145.

Mendoza, C., 2000. TOPbase/TIPbase, in *ATOMIC AND MOLECULAR DATA AND THEIR APPLICATIONS*, vol. 543 of **AIP Conference Proceedings**, pp. 313–315, Queens Univ, Theoret & Computat Phys Res Div, Sch Math & Phys; Int Union Pure & Appl Phys; NIST, Phys Lab; NIST, Atom Phys Div; NIST, Stand Reference Data Program, 2nd International Conference on Atomic and Molecular Data and their Applications (ICAMDATA 2000), KEBLE COLL, OXFORD, ENGLAND, MAR 26-30, 2000.

Miles, B. M. & Wiese, W. L., 1969. Critically evaluated transition probabilities for Ba I and Ba II, NBS Technical Note 474.

Miller, M. H., 1968. *Thermally insensitive determinations of transition probabilities for Si I, Si II, P I, P II, S I, S II and Ar II*, Ph.D. thesis, University of Maryland, Technical Note BN-550.

Miller, M. H., Roig, R. A., & Bengston, R. D., 1971. Transition probabilities of P I, P II, and Cl I lines, *Phys. Rev. A*, **4**, 1709.

Miller, M. H., Wilkerson, T. D., Roig, R. A., & Bengston, R. D., 1974. Absolute transition probabilities for the 2p2 3P-2p3s 3P0 multiplet of neutral Carbon, *Phys. Rev. A*, **9**, 2312.
Minnhagen, L., 1973. Spectrum and the energy levels of neutral argon, Ar I, *J. Opt. Soc. Am.*, **63**, 1185–1198.
Moise, N. L., 1966. Absolute transition probabilities for the Cu I resonance lines, *ApJ*, **144**, 782.
Moity, J., 1978. Experimental oscillator strengths for Ni II lines, *A&A*, **64**, 165.
Morton, D. C., 2000. Atomic data for resonance absorption lines II. Wavelengths longward of the Lyman limit for heavy elements, *ApJS*, **130**, 403–436.
Morton, D. C., 2003. Atomic data for resonance absorption lines. III. Wavelengths longward of the Lyman limit for the elements hydrogen to gallium, *ApJS*, **149**, 205–238.
Morton, D. C. & Smith, W. H., 1973. A compilation of interstellar oscillator strengths, *A&AS*, **26**, 333.
Musielok, J., Bridges, J. M., Djurovic, S., & Wiese, W. L., 1996. Oscillator strengths for N II lines, including intersystem lines, and tests of the spectroscopic coupling scheme, *Phys. Rev. A*, **53**, 3122–3128.
Musielok, J., Pawelec, E., Griesmann, U., & Wiese, W. L., 1999. Atomic transition probabilities of F I spectral lines from 3s-3p and 3p-3d transition arrays, *Phys. Rev. A*, **60**, 947–955.
Nave, G. & Johansson, S., 2012. THE SPECTRUM OF Fe II, *ApJS*, **204**, 1.
Nave, G., Johansson, S., Learner, R. C. M., Thorne, A. P., & Brault, J. W., 1994. A New Multiplet Table for Fe i, *ApJS*, **94**, 221.
Newsom, G. H., 1966. Absorption spectrum of calcium vapour - 1660-2028 å, *Proc. Phys. Soc.*, **87**, 975.
Newsom, G. H., 1968. The absorption spectrum of Calcium vapor: 1660-2028 A, *ApJ*, **154**, 1095–1098.
Nicolaides, C., Sinanoglu, O., & Westhaus, P., 1971. Oscillator strengths for the transitions 4s2 1S-4snp 1P in Ca I, *Phys. Rev. A*, **4**, 1400.
Nilsson, A. E., Johansson, S., & Kurucz, R. L., 1991. The spectrum of singly ionized yttrium, Y II, *Phys. Scr.*, **44**, 226.
Nussbaumer, H. & Rusca, C., 1979. Forbidden transitions in the Carbon sequence, *A&A*, **72**, 129–133.
Pachucki, K., 2024. Finite nuclear mass correction to the hyperfine splitting in hydrogenic systems, *Phys. Rev. A*, **109**, 052822.
Palmeri, P. & Wyart, J.-F., 1999. Interpretation of energy levels and predicted transition probabilities in neutral technetium (Tc I), *J. Quant. Spectrosc. Radiat. Transf.*, **61**, 603–616.
Parkinson, W. H., Reeves, E., & Tomkins, F. S., 1976. Measurements of Sc I gf-values, *Proc. R. Soc. London, Ser. A*, **352**, 589.
Pavlenko, Y. V., Yurchenko, S. N., McKemmish, L. K., & Tennyson, J., 2020. Analysis of the TiO isotopologues in stellar optical spectra, *A&A*, **42**, A77.
Pelletier, S., Benneke, B., Ali-Dib, M., Prinoth, B., Kasper, D., Seifahrt, A., Bean, J. L., Debras, F., Klein, B., Bazinet, L., Hoeijmakers, H. J., Kesseli, A. Y., Lim, O., Carmona, A., Pino, L., Casasayas-Barris, N., Hood, T., & Stürmer, J., 2023. Vanadium oxide and a sharp onset of cold-trapping on a giant exoplanet, *Nature*, **619**(7970), 491–494.
Peterson, R. C. & Kurucz, R. L., 2014. New Fe I Level Energies and Line Identifications from Stellar Spectra, *ApJS*, **216**, 1.
Peterson, R. C. & Kurucz, R. L., 2022. New Fe I Level Energies and Line Identifications from Stellar Spectra. III. Initial Results from UV, Optical, and Infrared Spectra, *ApJS*, **260**, 28.
Pezoa, F., Reutter, J. L., Suarez, F., Ugarte, M., & Vrgoč, D., 2016. Foundations of JSON schema, in *Proceedings of the 25th international conference on World Wide Web*, pp. 263–273.
Pfennig, H., Steele, R., & Trefftz, E., 1965. The Hartree-Fock approximation for Be I, B II, C III, *J. Quant. Spectrosc. Radiat. Transf.*, **5**, 335.
Pinnington, E. H., Irwin, D. J. G., Livingston, A. E., & Kernahan, J. A., 1976. Mean-life measurements for levels in F III, F IV and F V, *Can. J. Phys.*, **54**, 1014.
Podobedova, L. I., Kelleher, D. E., & Wiese, W. L., 2009. Critically evaluated atomic transition probabilities for sulfur S I–S XV, *J. Phys. Chem. Ref. Data*, **38**, 171–439.
Poulizac, M. C., Druetta, M., & Ceyzerat, P., 1971. Mean-life measurements in N II, N III and N IV, *J. Quant. Spectrosc. Radiat. Transf.*, **11**, 1087.
Prinoth, B., Seidel, J. V., Hoeijmakers, H. J., Morris, B. M., Baratella, M., Borsato, N. W., Damasceno, Y. C., Parmentier, V., Kitzmann, D., Sedaghati, E., Pino, L., Borsa, F., Allart, R., Santos, N., Steiner, M., Suárez Mascareño, A., Tabernero, H., & Zapatero Osorio, M. R., 2025. Titanium chemistry of WASP-121 b with ESPRESSO in 4-UT mode, *A&A*, **694**, A284.
Quinet, P., Palmeri, P., Fivet, V., Biémont, E., Nilsson, H., Engström, L., & Lundberg, H., 2008. Laser-induced-fluorescence lifetime measurements and relativistic Hartree-Fock oscillator strength calculations in singly ionized platinum, *Phys. Rev. A*, **77**, 022501.
Raassen, A. J. J., Pickering, J. C., & Uylings, P. H. M., 1998. Calculated oscillator strengths of singly ionized cobalt, *Astron. Astrophys., Suppl. Ser.*, **130**, 541–549.
Radžiūtė, L., Gaigalas, G., Kato, D., Rynkun, P., & Tanaka, M., 2020. Extended Calculations of Energy Levels and Transition Rates for Singly Ionized Lanthanide Elements. I. Pr–Gd, *ApJS*, **248**, 17.
Radžiūtė, L., Gaigalas, G., Kato, D., Rynkun, P., & Tanaka, M., 2021. Extended Calculations of Energy Levels and Transition Rates for Singly Ionized Lanthanide Elements. II. Tb-Yb, *ApJS*, **257**, 29.
Radziemski, L. J. & Kaufman, V., 1969. Wavelengths, Energy Levels, and Analysis of Neutral Atomic Chlorine (Cl I), *J. Opt. Soc. Am.*, **59**, 424–443.
Radziemski, L. J. & Kaufman, V., 1974. Wavelengths, energy levels, and analysis of the second spectrum of chlorine (Cl II)*, *J. Opt. Soc. Am.*, **64**, 366–389.
Ralchenko, Y., 2024a. Atomic Spectroscopy - Different Coupling Schemes, https://www.nist.gov/pml/atomic-spectroscopy-compendium-basic-ideas-notation-data-and-formulas/atomic-spectroscopy-2, Accessed: 01-March-2025.
Ralchenko, Y., 2024b. NIST Atomic Spectra Database, https://www.nist.gov/pml/atomic-spectra-database, Accessed: 01-June-2024.
Ralchenko, Y. & Kramida, A., 2020. Development of NIST atomic databases and online tools, *Atoms*, **8**, 56.
Roberts, J. R., Voigt, P. A., & Czernichowski, A., 1975. Experimental total probabilities for transitions of Ti II, *ApJ*, **197**, 791.
Roig, R. A., 1975. Absorption spectrum of Al I in the vacuum ultraviolet, *J. Phys.B-At. Mol. Phys.*, **8**, 2939–2947.
Roig, R. A. & Miller, M. H., 1979. Experimental transition probabilities for Cu II and Ag II, *J. Opt. Soc. Am.*, **64**, 1479.
Ryabchikova, T., Piskunov, N., Kurucz, R. L., Stempels, H. C., Heiter, U., Pakhomov, Y., & Barklem, P. S., 2015. A major upgrade of the VALD database, *Phys. Scr.*, **90**, 054005.
Ryabtsev, A. N., Kink, I., Awaya, Y., Ekberg, J. O., Mannervik, S., ölme, A., & Martinson, I., 2005. Additions to the Spectrum and Energy Levels and a Critical Compilation of Singly-Ionized Boron, B II, *Phys. Scr.*, **71**, 489.
Safronova, M. S., Safronova, U. I., & Clark, C. W., 2015. Correlation effects in La, Ce, and lanthanide ions, *Phys. Rev. A*, **91**, 022504.
Sahoo, B. K., Wansbeek, L. W., Jungmann, K., & Timmermans, R. G. E., 2009. Light shifts and electric dipole matrix elements in Ba^+ and Ra^+, *Phys. Rev. A*, **79**, 052512.
Salih, S. & Lawler, J. E., 1985. Radiative lifetimes of excited states in Ru I, *J. Opt. Soc. Am. B*, **2**, 422–425.
Salih, S., Duquette, D. W., & Lawler, J. E., 1983. Radiative lifetimes of the 5d3 6s 6p levels in Ta I, *Phys. Rev. A*, **27**, 1193–1196.
Saloman, E. B., 2004. Energy Levels and Observed Spectral Lines of Xenon, Xe I through Xe LIV, *J. Phys. Chem. Ref. Data*, **33**, 765–921.

Saloman, E. B., 2006. Wavelengths, Energy Level Classifications, and Energy Levels for the Spectrum of Neutral Mercury, *J. Phys. Chem. Ref. Data*, **35**, 1519–1548.
Saloman, E. B., 2007. Energy Levels and Observed Spectral Lines of Krypton, Kr I through Kr XXXVI, *J. Phys. Chem. Ref. Data*, **36**, 215–386.
Saloman, E. B., 2010. Energy Levels and Observed Spectral Lines of Ionized Argon, ArII through ArXVIII, *J. Phys. Chem. Ref. Data*, **39**, 033101.
Saloman, E. B., 2012a. Energy Levels and Observed Spectral Lines of Neutral and Singly Ionized Titanium, Ti I and Ti II, *J. Phys. Chem. Ref. Data*, **41**, 013101–013101–116.
Saloman, E. B., 2012b. Energy Levels and Observed Spectral Lines of Neutral and Singly Ionized Chromium, Cr I and Cr II, *J. Phys. Chem. Ref. Data*, **41**, 043103.
Saloman, E. B. & Kramida, A., 2017a. Critically evaluated energy levels, spectral lines, transition probabilities, and intensities of singly ionized vanadium (V II), *ApJS*, **231**, 19.
Saloman, E. B. & Kramida, A., 2017b. Critically evaluated energy levels, spectral lines, transition probabilities, and intensities of neutral vanadium (V I), *ApJS*, **231**, 18.
Saloman, E. B. & Sansonetti, C. J., 2005. Wavelengths, Energy Level Classifications, and Energy Levels for the Spectrum of Neutral Neon, *J. Phys. Chem. Ref. Data*, **33**, 1113–1158.
Sansonetti, C. J. & Reader, J., 2001. Spectrum and Energy Levels of Singly-Ionized Mercury (Hg II), *Phys. Scr.*, **63**, 219.
Sansonetti, J. E., 2006. Wavelengths, transition probabilities, and energy levels for the spectra of rubidium (Rb I through Rb XXXVII), *J. Phys. Chem. Ref. Data*, **35**, 301–421.
Sansonetti, J. E., 2007. Spectroscopic Data for Neutral Francium (FrI), *J. Phys. Chem. Ref. Data*, **36**, 497–507.
Sansonetti, J. E., 2008a. Wavelengths, Transition Probabilities, and Energy Levels for the Spectra of Sodium (NaI–NaXI), *J. Phys. Chem. Ref. Data*, **37**, 1659–1763.
Sansonetti, J. E., 2008b. Wavelengths, transition probabilities, and energy levels for the spectra of potassium (K I through K XIX), *J. Phys. Chem. Ref. Data*, **37**, 7–96.
Sansonetti, J. E., 2009. Wavelengths, transition probabilities, and energy levels for the spectra of cesium (Cs I–Cs LV), *J. Phys. Chem. Ref. Data*, **38**, 761–923.
Sansonetti, J. E., 2012. Wavelengths, transition probabilities, and energy levels for the spectra of strontium ions (Sr II through Sr XXXVIII), *J. Phys. Chem. Ref. Data*, **41**, 013102.
Sansonetti, J. E. & Martin, W. C., 2005. Handbook of Basic Atomic Spectroscopic Data, *J. Phys. Chem. Ref. Data*, **34**, 1559–2259.
Sansonetti, J. E. & Nave, G., 2010. Wavelengths, transition probabilities, and energy levels for the spectrum of neutral strontium (Sr I), *J. Phys. Chem. Ref. Data*, **39**, 033103.
Schaefer, A. R., 1971. Lifetimes of excited states in Mg I, Ca I, Sr I, Ba I and Y I, *ApJ*, **163**, 411.
Schenhage, S. E., Danzmann, K., Kunnemeyer, R., & Kock, M., 1983. Experimental transition probabilities for Mo I and Mo II lines, *J. Quant. Spectrosc. Radiat. Transf.*, **29**, 507–516.
Schulz-Gulde, E., 1969. Transition probabilities for Si I lines, *J. Quant. Spectrosc. Radiat. Transf.*, **9**, 13.
Seaton, M. J., 1998. Oscillator strengths in Ne I, *J. Phys. B-At. Mol. Opt. Phys.*, **31**, 5315–5336.
Seaton, M. J., 2005. Opacity Project data on CD for mean opacities and radiative accelerations, *MNRAS*, **362**, L1–L3.
Sengupta, S., 1975. Oscillator strengths for the Li I isoelectronic sequence, *J. Quant. Spectrosc. Radiat. Transf.*, **15**, 159.
Shackleford, W. L., 1965. Transition probabilities for the resonance lines of Cr I and Cr II, *J. Quant. Spectrosc. Radiat. Transf.*, **5**, 303.
Shang, X., Wang, Q., Tian, Y.-S., Wang, C., & Dai, Z.-W., 2015. Radiative lifetimes, branching fractions, transition probabilities and oscillator strengths of some levels for neutral yttrium, *J. Phys. B-At. Mol. Opt. Phys.*, **48**, 085001.
Shirai, T., Reader, J., Kramida, A. E., & Sugar, J., 2007. Spectral Data for Gallium: Ga I through Ga XXXI, *J. Phys. Chem. Ref. Data*, **36**, 509–615.
Simonnin, A., Parmentier, V., Wardenier, J. P., Chauvin, G., Chiavassa, A., N'Diaye, M., Tan, X., Bean, J., Line, M., Kitzmann, D., Kasper, D., Seifhart, A., Brogi, M., Lee, E. K. H., Pelletier, S., Pino, L., Prinoth, B., Seidel, J. V., Weiner Mansfield, M., Benneke, B., Désert, J.-M., Gandhi, S., Hammond, M., Palma-Bifani, P., Rauscher, E., & Smith, P., 2024. Time Resolved Absorption of Six Chemical Species With MAROON-X Points to Strong Drag in the Ultra Hot Jupiter TOI-1518 b, *A&A*, **698**, A314.
Sinanoglu, O., 1973. Theory of atomic lifetimes, *Nuclear Inst. and Methods*, **110**, 193.
Smith, M. W. & Wiese, W. L., 1971. Graphical presentations of systematic trends of atomic oscillator strengths, *ApJS*, **23**, 103.
Smith, P. L. & Kuhne, M., 1978. Oscillator strengths of Cr I lines lying between 200 and 541 nm, *Proc. R. Soc. London, Ser. A*, **363**, 263.
Smith, W. H. & Liszt, H. S., 1971. Absolute oscillator strengths for some resonance transitions of Mg I, Mg II, Al I, Si II and Si IV, *J. Opt. Soc. Am.*, **61**, 938.
Spake, J. J., Sing, D. K., Evans, T. M., Oklopcic, A., Bourrier, V., Kreidberg, L., Rackham, B. V., Irwin, J., Ehrenreich, D., Wyttenbach, A., Wakeford, H. R., Zhou, Y., Chubb, K. L., Nikolov, N., Goyal, J. M., Henry, G. W., Williamson, M. H., Blumenthal, S., Anderson, D. R., Hellier, C., Charbonneau, D., Udry, S., & Madhusudhan, N., 2018. Helium in the eroding atmosphere of an exoplanet, *Nature*, **557**, 68+.
Stuck, D. & Wende, B., 1974. Measurement of transition probabilities of C I transitions in the vacuum ultraviolet, *Phys. Rev. A*, **9**, 1–8.
Sugar, J. & Corliss, C., 1985. Atomic energy levels of the iron-period elements: potassium through nickel, Tech. rep., American Chemical Society, Washington, DC.
Sugar, J. & Musgrove, A., 1988. Energy Levels of Molybdenum, Mo I through Mo XLII, *J. Phys. Chem. Ref. Data*, **17**, 155–239.
Sugar, J. & Musgrove, A., 1990. Energy Levels of Copper, Cu I through Cu XXIX, *J. Phys. Chem. Ref. Data*, **19**, 527–616.
Sugar, J. & Musgrove, A., 1993. Energy Levels of Germanium, Ge I through Ge XXXII, *J. Phys. Chem. Ref. Data*, **22**, 1213–1278.
Sugar, J. & Musgrove, A., 1995. Energy Levels of Zinc, Zn I through Zn XXX, *J. Phys. Chem. Ref. Data*, **24**, 1803–1872.
Sun, Y., Hu, F., Li, W., Liu, D., Mei, M., & Gou, B., 2021. Energy levels and transition probabilities of N^{+}, F^{3+}, and Ne^{4+} ions, *Zeitschrift für Naturforschung A*, **76**, 1–12.
Tatum, J. B., 1968. The solar abundance of Cobalt, *MNRAS*, **140**, 87.
Tennyson, J. & Yurchenko, S. N., 2012. ExoMol: molecular line lists for exoplanet and other atmospheres, *MNRAS*, **425**, 21–33.
Tennyson, J., Hill, C., & Yurchenko, S. N., 2013. Data structures for ExoMol: Molecular line lists for exoplanet and other atmospheres, in *6^{th} international conference on atomic and molecular data and their applications ICAMDATA-2012*, vol. 1545 of **AIP Conference Proceedings**, pp. 186–195, AIP, New York.
Tennyson, J., Pezzella, M., Zhang, J., & Yurchenko, S. N., 2023. Data structures for photoadsorption within the ExoMol project, *RASTI*, **2**, 231–237.
Tennyson, J., Yurchenko, S. N., Zhang, J., Bowesman, C. A., Brady, R. P., Buldyreva, J., Chubb, K. L., Gamache, R. R., Gorman, M. N., Guest, E. R., Hill, C., Kefala, K., Lynas-Gray, A. E., Mellor, T. M., McKemmish, L. K., Mitev, G. B., Mizus, I. I., Owens, A., Peng, Z., Perri, A. N., Pezzella, M., Polyansky, O. L.,

Qu, Q., Semenov, M., Smola, O., ov, A., Somogyi, W., Upadhyay, A., Wright, S. O. M., & Zobov, N. F., 2024. The 2024 release of the ExoMol database: molecular line lists for exoplanet and other hot atmospheres, *J. Quant. Spectrosc. Radiat. Transf.*, **326**, 109083.

Tidwell, E. D., 1972. Transition probabilities in Ne I, *J. Quant. Spectrosc. Radiat. Transf.*, **12**, 431–441.

Trimble, W. L., Sulai, I. A., Ahmad, I., Bailey, K., Graner, B., Greene, J. P., Holt, R. J., Korsch, W., Lu, Z.-T., Mueller, P., & O'Connor, T. P., 2009. Lifetime of the 7s6d $^1D_2$ atomic state of radium, *Phys. Rev. A*, **80**, 054501.

van Kleef, T. A. M. & Metsch, B. C., 1978. Term analysis of singly ionized iridium (Ir II), *Physica B+C*, **95**, 251–265.

Vergès, J. & Wyart, J.-F., 1978. Infrared Emission Spectrum of Lutecium and Extended Analysis of Lu I, *Phys. Scr.*, **17**, 495.

Vidolova-Angelova, E., Baharis, C., Roupakas, G., & Kompitsas, M., 1996. Observations and theoretical analysis of highly excited singlet and triplet states of cadmium, *Journal of Physics B: Atomic, Molecular and Optical Physics*, **29**, 2453.

Wahlgren, G. M., Brage, T., Brandt, J. C., Fleming, J., Johansson, S., Leckrone, D. S., Proffitt, C. R., Reader, J., & Sansonetti, C. J., 2001. The Bismuth Abundance in the HgMn Stars χ Lupi and HR 7775 and Improved Atomic Data for Selected Transitions of Bi I, Bi II, and Bi III, *ApJ*, **551**, 520.

Wang, R., 2024. *ExoMol format atomic line lists based on the NIST database*, Master's thesis, University College London.

Warner, B., 1967. Absolute oscillator strengths for Ti II, *Mem.RAS*, **70**, 165.

Warner, B., 1968a. Atomic oscillator strengths in Al I, Si I, P I, S I and Ca I, *MNRAS*, **140**, 53–59.

Warner, B., 1968b. Atomic oscillator strengths in Mg, Al, Si, P, S, Cl and Ar, *MNRAS*, **139**, 103.

Warner, B., 1968c. Transition probabilities in the spectra of Alkali-like atoms, *MNRAS*, **139**, 115–128.

Weiss, A. W., 1975. Theoretical oscillator strengths for the Al I isoelectronic sequence, *Phys. Rev. A*, **9**, 1524–1536.

Werbowy, S. & Kwela, J., 2009. The E2 admixtures in mixed multipole lines 459.7 and 564.0 nm of Bi I, *Can. J. Phys.*, **87**, 851–856.

Whaling, W. & Brault, J. W., 1988. Comprehensive transition probabilities in Mo I, *Phys. Scr.*, **38**, 707–718.

Whaling, W., Martinez-Garcia, M., Mickey, D. L., & Lawrence, G. M., 1970. Lifetimes and oscillator strengths for Fe I, *Nucl. Instrum. Methods*, **99**, 363.

Whaling, W., Hannaforn, P., Lowe, R. M., Biemont, E., & Grevesse, N., 1984. Lifetimes and oscillator strengths for Mo I, *J. Quant. Spectrosc. Radiat. Transf.*, **32**, 69–80.

Wickliffe, M. E. & Lawler, J. E., 1997a. Atomic transition probabilities for Tm I and Tm II, *J. Opt. Soc. Am. B*, **14**, 737–753.

Wickliffe, M. E. & Lawler, J. E., 1997b. Atomic transition probabilities for Ni I, *ApJS*, **110**, 163–166.

Wiese, W. L. & Fuhr, J. R., 1975. Atomic transition probabilities for Scandium and Titanium, *J. Phys. Chem. Ref. Data*, **4**, 263.

Wiese, W. L. & Fuhr, J. R., 2007. Improved critical compilations of selected atomic transition probabilities for neutral and singly ionized carbon and nitrogen, *J. Phys. Chem. Ref. Data*, **36**, 1287–1345.

Wiese, W. L. & Fuhr, J. R., 2009. Accurate atomic transition probabilities for hydrogen, helium, and lithium, *J. Phys. Chem. Ref. Data*, **38**, 565–726.

Wiese, W. L. & Martin, G. A., 1980. Transition probabilities, in *Wavelengths and Transition Probabilities for Atoms and Atomic Ions, Nat. Stand. Ref. Data Ser. NSRDS-68*, Nat. Bur. Stand., U.S.

Wiese, W. L. & Martin, G. A., 1989. Atomic transition probabilities, in *CRC Handbook of Chemistry and Physics, 70th Edition*, eds Weast, R. C., Lide, D. R., Astle, M. J., & Beyer, W. H., CRC Press, Boca Raton, FL.

Wiese, W. L., Smith, M. W., & Glennon, B. M., 1966. Atomic transition probabilities, Vol. I: Hydrogen through neon – A critical data compilation, in *Nat. Stand. Ref. Data Ser., NSRDS-NBS 4*, U.S. Government Printing Office, Washington, D.C.

Wiese, W. L., Smith, M. W., & Miles, B. M., 1969. Atomic transition probabilities, Vol. II: Sodium through calcium - A critical data compilation, in *Nat. Stand. Ref. Data Ser., NSRDS-NBS 22*, U.S. Government Printing Office, Washington, D.C.

Wiese, W. L., Fuhr, J. R., & Deters, T. M., 1996. *Atomic transition probabilities of carbon, nitrogen, and oxygen – A critical data compilation, J. Phys. Chem. Ref. Data, Monograph No. 7*, AIP Press, Melville, NY.

Wolnik, S. J. & Berthel, R. O., 1973. Shock-tube measurements of absolute gf-values for Ti I and Ti II, *ApJ*, **179**, 665.

Wolnik, S. J., Berthel, R. O., Carnevale, E. H., & Wares, G. W., 1969. Shock-tube measurements of absolute gf-values for Cr I and Cr II, *ApJ*, **157**, 983.

Wolnik, S. J., Berthel, R. O., & Wares, G. W., 1971. Shock-tube measurements of absolute gf-values for Fe I, *ApJ*, **166**, L31.

Wood, D. R. & Andrew, K. L., 1968. Arc Spectrum of Lead*, *J. Opt. Soc. Am.*, **58**, 818–829.

Woodyard, J. & Altick, P. L., 1979. Ab initio configuration interaction calculation of the 1S0-3P1 transition in Ar I, *J. Phys. B-At. Mol. Opt. Phys.*, **7**, 2298.

Wujec, T., Baclawski, A., Golly, A., & Ksiazek, I., 1999. Studies of the bromine spectrum and determination of transition probabilities for Br I and Br II lines, *Acta Phys. Pol. A*, **96**, 333–340.

Wyart, J.-F., Blaise, J., & Joshi, Y. N., 1995. Theoretical study of the odd parity levels and transition probabilities in Pt II, *Phys. Scr.*, **52**.

Xie, T., 2024. *ExoMol format atomic line list based on the Kurucz Database*, Master's thesis, University College London.

Xu, H. L., Persson, A., Svanberg, S., Blagoev, K., Malcheva, G., Pentchev, V., Biémont, E., Campos, J., Ortiz, M., & Mayo, R., 2004. Radiative lifetime and transition probabilities in Cd I and Cd II, *Phys. Rev. A*, **70**, 042508.

Xu, H. L., Svanberg, S., Quinet, P., Palmeri, P., & Biémont, E., 2007. Improved atomic data for iridium atom (Ir I) and ion (Ir II) and the solar content of iridium, *J. Quant. Spectrosc. Radiat. Transf.*, **104**, 52–70.

Yerokhin, V. A. & Shabaev, V. M., 2015. Lamb Shift of n = 1 and n = 2 States of Hydrogen-like Atoms, $1 \leq Z \leq 110$, *J. Phys. Chem. Ref. Data*, **44**, 033103.

Younger, S. M., Fuhr, J. R., Martin, G. A., & Wiese, W. L., 1978. Atomic transition probabilities for Vanadium, Chromium, and Manganese, *J. Phys. Chem. Ref. Data*, **7**, 495.

Zhang, J., Tennyson, J., & Yurchenko, S. N., 2024. PyExoCross: a Python program for generating spectra and cross-sections from molecular line lists, *RASTI*, **3**, 257–287.

APPENDIX A: EXAMPLE ADEF.JSON FILE FOR THE H MOLECULE


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


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