

DIVISION B
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**ATOMIC AND MOLECULAR
DATA**

*DONNÉES ATOMIQUES
ET MOLÉCULAIRES*

WORKING GROUP

ATOMIC DATA
DONNÉES ATOMIQUES

CHAIR
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This report summarizes laboratory measurements of atomic wavelengths, energy levels, hyperfine and isotope structure, energy level lifetimes, and oscillator strengths. Theoretical calculations of lifetimes and oscillator strengths are also included. The bibliography is limited to species of astrophysical interest. Compilations of atomic data and internet databases are also included. Papers are listed in the bibliography in alphabetical order, with a reference number in the text.

Comprehensive lists of references for atomic spectra can be found in the NIST Atomic Spectra Bibliographic Databases <http://physics.nist.gov/asbib>.

1. Energy levels, wavelengths, line classifications, and line structure

Major analyses of wavelengths, energy levels and line classifications have been published for **Cr II**[274, 275], **Fe II**[227], and **V II**[311] in the past three years. Laboratory wavelengths and line identifications have been published for coronal lines observed in spectra from the Solar Dynamics Observatory in the region 193 Å to 218 Å and around 131 Å [38, 312, 313]. Wavelengths and identifications of additional coronal lines between 170 Å and 291 Å have been measured using the Hinode EUV Imaging Spectrometer [64].

Additional publications of wavelengths, energy levels, line classifications, hyperfine structure (HFS), and isotope structure (IS) include:

Al II (HFS): [26], **Ar IX**: [277], **B II**: [208], **Br III**: [140], **Cl I**: [300], **Co II** (forbidden): [256], **Dy I**: [292], **Eu I** (HFS,IS): [2, 102, 103, 104], **Fe VIII-IX**: [230], **Fe VIII-XVI**: [37], **Fe XI**: [66], **Fe XIII**: [62], **Fe XVI**: [36], **Fe XVII**: [63], **Fe XVIII**: [54], **Fe XVIII-XXV**: [254], **Gd I** (IS,HFS): [145], **I I**: [124], **K I**: [51], **K III**: [22], **La I**: [106], **Li I**: [50], **Mg VII-VIII**: [177], **Mn I** (HFS): [25, 165], **Mn II**: [46], **N III**: [112], **Na I**: [52], **Nb I**: [72, 235], **Nb I** (HFS): [95], **Nd II** (HFS): [28], **Ne IV**: [170], **Ni I**: [288, 291], **O I**: [204], **O VI**: [341], **P II**: [153], **Pr I** (HFS): [107, 282, 319], **Pr II**: [21], **Pr II** (HFS): [20], **Ru I** (IS,HFS): [101], **S I**: [153], **S VII-XIV**: [180], **S VIII**: [237], **Si IV**: [220], **Se III**: [305], **Sm I**: [174], **Sn II**: [128], **Sn III**: [129], **Ta II**: [318], **Te III**: [306], **Ti X**: [7], **Ti IV**: [220], **Tl I** (IS,HFS): [246], **V I** (HFS): [121, 122, 123], **V II** (forbidden): [256], **V II** (HFS): [1, 29], **Zn I**: [49] **Zn II**: [220].

The references included here for elements heavier than Ni ($Z > 28$) are limited to the first three spectra only, these data being of most interest for astronomical spectroscopy.

Analyses of neutral through doubly-ionized iron-group spectra using Fourier transform spectroscopy (FTS) and grating spectroscopy are underway at the National Institute of Standards and Technology (NIST), USA and Imperial College London, UK. Analysis of moderately ionized species (III-VIII) is being done at NIST, USA; Observatoire de Paris-Meudon, France; the Institute of Spectroscopy in Troitsk, Russia; Centro Investigaciones Opticas, La Plata, Argentina; and Aligarh Muslim University, India. Measurements of HFS and IS using both FTS and laser spectroscopy are in progress at Istanbul University, Turkey; Lund University, Sweden; Graz University of Technology, Austria; Instituut voor Kern- en Stralingsfysica, Leuven, Belgium; Bhabha Atomic Research Centre, India; Poznań University of Technology, Poland; University of Birmingham, UK; ISOLDE (international collaboration including Switzerland, Germany, France, UK, Russia, Belgium, Spain, Portugal, and Japan); and York University, Toronto, Canada.

Studies of more highly-ionized elements are being done using electron beam ion traps (EBIT) at NIST, USA; Lawrence Livermore National Laboratory, USA; Heidelberg, Germany; Shanghai, China; with an accelerator in Beijing, China; and at the National Institute for Fusion Science, Japan.

Theoretical calculations of energy levels, oscillator strengths, HFS, IS, photoionization, and collisional data are currently being performed at NIST, USA; Ohio State University, USA; Queens University Belfast, Northern Ireland; and the University of Lund, Sweden.

2. Wavelength standards

The thorium-argon hollow cathode lamp is an important calibration source for ground-based astronomical spectrographs and new Ritz wavelengths for 19874 thorium lines measured using FTS have been published [248]. In the infrared, uranium-neon hollow cathode lamps have advantages over thorium-argon lamps and an atlas based on FTS for the U/Ne lamp between 850 and 4000 nm has been published [249]. The calibration of these FTS measurements included reference lines in U and Th measured using optical-galvanic spectroscopy [61]. Additional Ritz wavelengths based on FTS have been published for Fe II, Mg I-II, Cr II, Ti II, Mn II, Ni II, and Zn II [226]. Wavenumbers and pressure shifts in Ar have been measured using laser spectroscopy [322].

In more highly-charged ions, laser spectroscopy measurements of the $2p^2 P_{3/2} - 2^2 P_{1/2}$ forbidden transition in Ar XIV has been performed in an EBIT [194]. High-accuracy wavelength standards in the 3 keV region have been published for lines of S XIII-XV, Cl XIV-XV, and Ar XV-XVII [281].

3. Oscillator strengths

The transition-probability data in the references in section 9 were obtained by both theoretical and experimental methods. The references included here for elements heavier than Ni ($Z > 28$) are limited to the first three or four spectra only. For Fe II, the set of critically evaluated oscillator strengths has been greatly expanded in the NIST Atomic Spectra Database (<http://physics.nist.gov/asd>) and now contains data for 6700 Fe II lines from 92 nm to 87 μm . Extensive sets of oscillator strengths of fine structure levels ($n \leq 10$) are being calculated with the Breit-Pauli R-matrix (BPRM) method by S. Nahara, Ohio State Univ, USA (see NORAD database in section 6).

4. Photoionization cross-sections

Many of the theoretical papers in the references also include data on photoionization and collisional cross-sections. Additional references for both experimental and calculated cross-sections are as follows:

Al V: 186	Fe II: 100	Ne VIII: 343
Al X: 187	Fe X: 16	Ni I: 288
Ar VI: 178	Fe XV: 161	O II-III: 41
Ar IX: 108	Fe XVII: 108	P III-IV: 135
B II: 208	Ga I: 139	S IX: 317
Be I: 134	Ge I: 27	S V: 163
C II: 207	K III: 22	Se II: 203
C IV: 193	Kr II: 202, 270	Si IX: 317
Ca II: 297	N III: 112	Sr I: 78
Ca XI: 185	N IV-V: 289	Ti XIX: 188
Cl I: 300, 339	N IV : 162	Ti XX: 189
Cu XX: 184	Ne VII : 162	

5. Compilations, Reviews, Conferences

Major compilations of wavelengths, energy levels or oscillator strengths have been published for the following: **Ag II**: [166], **Cr I-II**: [271, 274], **Fe II**: [227], **Fe V**: [169], **In II**: [168], **Mn II**: [171], **Ne IV**: [170], **Sn II**: [128], **Sr II**: [276], **Ti I-II**: [272]. A summary of the methods used for the critical evaluation of atomic data is given in [167].

Papers on atomic spectroscopic data are included in the proceedings of the 11th International Conference on Atomic Spectra and Oscillator Strengths [244] and the 8th International Conference on Atomic and Molecular Data and their Applications [113]. Additional meetings including papers on atomic data include the meetings of the Laboratory Astrophysics Division (LAD) of the American Astronomical Society (AAS), the International Conference on Atomic Processes in Plasmas, the Congress of the European Group on Atomic Systems, the International Conference on Phenomena in Ionized Gases; and the meeting of the Division of Atomic, Molecular and Optical Physics of the American Physical Society.

6. Databases

The following databases of atomic spectra at NIST have received significant updates since the last triennial report:

NIST Atomic Spectra Database, Version 5 (Sept 2014):

<http://physics.nist.gov/asd> contains critically compiled data on wavelengths, energy levels and oscillators strengths.

NIST Atomic Spectra Bibliographic Databases: (Frequently updated)

<http://physics.nist.gov/asbib> consists of three databases of publications on atomic transition probabilities, atomic energy levels and spectra, and atomic spectral line broadening.

Additional on-line databases including significant quantities of atomic data include:

NIST Database of Basic Atomic Spectroscopic Data, Version 1.1.3, (Nov 2013) <http://physics.nist.gov/handbook> Provides a selection of the most important and frequently used atomic spectroscopic data in an easily accessible format.

The MCHF/MCDHF Collection on the Web, Version 2 (Sept 2010) (C.Froese Fischer *et al.*) at <http://nlte.nist.gov/MCHF/index.html> contains results of multi-configuration Hartree-Fock (MCHF) or Dirac-Hartree-Fock (MCDHF) calculations for hydrogen and Li-like through Ar-like ions, mainly for $Z \leq 30$.

TOPbase, TIPbase, and OPserver (Feb, 2009)

<http://cdsweb.u-strasbg.fr/topbase/testop/home.html> provides links to databases of atomic data from the Iron Project and Opacity Projects, with an emphasis on data for astrophysically abundant ions ($Z \leq 26$).

NORAD-Atomic-Data (Dec, 2013)

http://www.astronomy.ohio-state.edu/~nahar/nahar_radiativeatomicdata/index.html includes more recent data from the Opacity and Iron Projects.

CHIANTI, version 7.1.4 (May, 2014), <http://www.chiantidatabase.org/> contains atomic data and programs for computing spectra of astrophysical plasmas, with the emphasis on highly-ionized atoms.

AtomDB, version 3.0.0 (Beta 4, Aug, 2014), <http://www.atomdb.org> is an atomic database for X-ray plasma spectral modeling, with the main emphasis being the modeling of collisional plasmas.

The Vienna Atomic Line Database (VALD3), (Feb, 2014)

<http://vald.astro.uu.se> is a database that aims to compile complete lists of spectral line parameters relevant to the interpretation of stellar atmospheric spectra.

The BIBL database, version 1.58.5 (March, 2014)

<http://das101.isan.troitsk.ru/bibl.htm> is a comprehensive bibliographic database of experimental and theoretical papers on atomic spectroscopy, with an emphasis on papers published since 1983.

The Virtual Atomic and Molecular Data Centre (VAMDC)

<http://www.vamdc.eu> provides a uniform access to a large number of atomic and molecular databases related to astrophysics.

7. Data Needs

Atomic data needs have been summarized in white papers from the AAS Laboratory Astrophysics Working Group (now LAD) [338]. In this section, a few important atomic data needs either for upcoming missions or in support of recent analyses of astrophysical spectra are highlighted.

New ground-based and space-based infrared (IR) spectrographs such as the Stratospheric Observatory for Infrared Astronomy (SOFIA), the Apache Point Observatory Galactic Evolution Experiment (APOGEE), and the Cryogenic High-resolution Infrared Echelle Spectrograph (CRIRES) have increasing demands for atomic data. The wavelength calibration above $2.5 \mu\text{m}$ is particularly problematic and new wavelength standards in either atomic or molecular species are needed. Measured oscillator strengths in the IR are limited to Fe I, Ti I, and a handful of lines for other species. Additional data are particularly needed in the H-band (around $1.5 \mu\text{m}$). The measurement of these oscillator strengths is challenging due to the high excitation of the upper energy level of many of the transitions giving lines in this wavelength region.

Smith & Brickhouse [293] summarize atomic data needs in X-ray astronomy. The interpretation of data from the Chandra X-ray Observatory's Low-Energy Transmission Grating (LETG) has been hampered by the lack of accurate wavelengths and collisional cross sections in the wavelength region from 50 \AA to 150 \AA . Spectra from the ASTRO-H SXS microcalorimeter, to be launched in 2015, are also likely to be affected. Also required is the improvement of the estimation of uncertainties in atomic data.

The astrophysical models used to measure the chemical abundances, evolution, and physical conditions in many astronomical objects require line identifications, wavelengths, oscillator strengths, collision strengths, photoionization cross sections, and recombination rate coefficients. Although high accuracy experimental wavelengths and oscillator strengths are frequently available for lines from low ionization stages, the measurement of oscillator strengths become more challenging for higher ionization stages of abundant elements. Improved theoretical calculations of moderate accuracy are thus needed, as are calculations of photoionization and collisional cross-sections. The large differences in abundances obtained from the collisional excitation lines of O III and recombination lines of O II observed in planetary nebulae has partially been resolved by improved calculations [238] and similar calculations for other ions are needed.

One notable example of the influence of new atomic data is the composition and opacity of the sun. A new analysis of elemental abundances in the solar spectrum resulted in reductions of 30-50 % in CNO abundances [31], but these revised abundances cannot be reconciled with standard models of the stellar interior using helioseismology. A potential resolution to this conflict would come from an increase in 15 % in the opacity of the solar plasmas. A new laboratory measurement of the iron opacity at conditions similar to those at the solar radiation/convection zone boundary provides an indication of this [35], with an opacity up to 4 times higher than predicted from atomic structure calculations. Since the principal contributors to the opacity are photo-excitation and photoionization, the new measurement indicates that improved calculations are needed for these processes for many abundant elements in the sun. Recent calculations for Fe XVII [217], show an increase of 20 % in opacity for this ion and new calculations for other iron ions are in progress.

8. Notes for References

The references are identified by a running number. This refers to the general reference list at the end of this report, where the literature is ordered alphabetically according to the first author. Each reference contains one or more code letters indicating the method applied by the authors, defined as follows:

THEORETICAL METHODS:

Q: quantum mechanical calculations. **QF:** Calculations of forbidden lines.

EXPERIMENTAL METHODS:

CL: New classifications

EL: Energy levels.

WL: Wavelengths.

HFS: Hyperfine structure.

IS: Isotope structure.

L: Lifetimes.

TE: Experimental oscillator strengths. **PI:** Photoionization cross-sections.

OTHER:

CP: Data compilations. **R:** Relative values only. **F:** Forbidden lines.

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9. References on lifetimes and oscillator strengths

Ag I : 32	Cu I : 32, 192	Li I : 57
Al II : 26	Eu I : 97, 146, 346	Lu I : 156
Al IV : 89	Eu II : 329, 346	Lu III : 159
Al X : 10	F I : 111	
Al XI : 57		Mg I : 48
Al XII : 5, 250	Fe I : 133, 200, 255, 257	Mg II : 114
	Fe II : 59, 60, 200, 286	Mg III-XI : 74
Ar II : 39, 97, 219	Fe VII : 310	Mg III : 24, 55, 89
Ar III : 44, 298	Fe VIII : 231, 309	Mg V : 308
Ar VI : 88	Fe IX : 70, 231	Mg VIII : 302
Ar XV : 91	Fe X : 68	Mg XI : 5
Ar XVI : 213, 223	Fe XI : 17, 66, 82	
Ar XVII : 213, 323	Fe XII : 69	Mn I : 25, 131, 154, 210, 285
	Fe XIII : 65	Mn II : 46, 131, 171
Ba II : 114	Fe XIV : 12, 96, 212	Mn XII : 87
	Fe XVI : 53, 77	Mn X-XIII : 315
Be II : 114, 115, 267	Fe XVII : 40, 53, 109, 217	Mn XXIV : 6
	Fe XVIII : 211	
C II : 294	Fe XXII : 86	Mo I : 143
C III : 278	Fe XXIII : 83, 278	Mo II : 141
C IV : 57, 206	Fe XXIV : 160, 223	Mo III : 240
	Fe XXV : 8	
Ca I : 48		N I : 332
Ca II : 19, 114	Ga II : 47	N II : 287, 340
Ca III : 23	Ga III : 80	N V : 206
Ca IX : 173		
Ca XIV : 79	Gd I-II : 98, 327, 330	Na I : 52
Ca XVIII : 160, 223		Na VII : 150
Ca XIX : 4	He I : 144	Na II-X : 75
Cd II : 114	Hf II : 42	Nb II : 251
Ce III : 320, 321	Hg II : 114	Nd I : 299
Cl I : 232	In I : O 264	Ne I : 30, 182, 239, 279
Cl II-V : 315		Ne II : 219
Cl III : 295	K I : 51, 222	Ne IV : 214, 215
Cl IV : 120	K XVI : 11	Ne V : 56
Cl XIV : 11	K XVIII : 4	Ne VI : 302
Cl XVI : 4		Ne VII : 76, 151, 278
	Kr I : 205	
Co XVIII-XXVI : 127	Kr II : 219	Ni I : 285, 337
Co II : 256		Ni II : 45
	La I : 99, 132, 283	Ni X : 268
Cr II : 33, 334	La II : 283	Ni XI : 67
Cr XII : 119	La III : 158	Ni XIV : 326
Cr XXIII : 6		Ni XV : 71, 85, 117, 172

Ni XVII : 138	Sc I : 236	Ti I : 175, 216
Ni XXI : 18	Sc II : 252	Ti II : 253, 336
Ni XXVI : 333	Sc III : 221, 263	Ti IV : 220
Ni XXVII : 225	Sc III-XXI : 201	Ti VI : 15
	Sc XX : 4	Ti VII : 290
O I : 229		Ti VII-X : 315
O II : 126	Si I : 110	Ti X : 7
O III : 229, 238, 301	Si II : 13	Ti XIX : 3
O IV : 228, 302	Si III : 344	Ti XX : 223
O V-VI : 90	Si IV : 220	Ti XXI : 6
O VI : 93, 206	Si IX : 335	
	Si V-XIII : 331	Tl I : 262
P VIII-X : 314	Si VII : 296	
P XIV : 5	Si VIII : 307, 314	U I : 58, 197
	Si X : 302	
Pb III : 261	Si XII : 223	V I : 328
		V II : 256
Re I : 234	Sm I : 130, 174	V XII : 118
Re II : 233	Sm II : 347	V XXII : 6
Rh I : 196	Sn I : 128, 142	W II : 176
Rh II : 34, 241	Sn III : 129	
		Xe II : 219
		Xe VI : 105, 247
Ru I : 342	Sr II : 114, 276	
		Y I : 284
S II : 164	Tb I : 195	Y III : 266
S VII : 94		
S VIII : 237	Te II-III : 348	
S IX,XI : 314		Yb I : 157
S IX-XII : 183	Th II : 136	
S XIII : 179, 280		Zn I : 47, 49, 191
S XV : 5		Zn II : 114, 220
		Zr II : 242, 243
He-like ions: 155, 245, 269	O-like ions: 259	
Li-like ions: 9, 73, 92, 224	Mg-like ions: 137, 265	
Be-like ions: 14, 116, 199, 273, 324	Ne-like ions: 148, 181, 277	
B-like ions: 149, 198, 258, 303, 304	Si-like ions: 84	
C-like ions: 81, 152, 190, 209, 316, 325, 345	F-like ions: 147, 218	
N-like ions: 125, 260	Neutral Li-Ar : 43	

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