

Session E

Comparison with observations

Atomic Physics Data for Stellar Atmospheres Research

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Abstract.

The review will cover the following topics: (1) Ionization energies; (2) Partition functions; (3) Sources of data for atomic and ionic wavelengths, transition probabilities, and broadening parameters, including nuclear effects (hfs and isotope shifts); (4) Opacities from photoionization of abundant elements (atoms and atomic ions) with emphasis on integration of TOPBASE material; and (5) Data bases for diatomic molecules. We emphasize topics of direct relevance to the synthesis of stellar spectra, primarily within the domain where LTE is useful. Additional parameters, such as line-broadening parameters, or excitation cross sections are not reviewed.

1. Ionization Energies

We provide a table of ionization energies from reliable secondary sources. First and second spectra are from the web pages of NIST (Sansonetti and Martin 2002). Most of the values for the third and fourth spectra are from the Handbook of Chemistry and Physics, 3rd Electronic Edition: (<http://www.hbcpnetbase.com/hbcp/>), but with a few additions from Dappen(2000) and Cowan (1981, Table 1-1). For the first and second spectra, only a few values differ by more than a few hundredths of an eV from those given by Moore (1970). Notable changes in the first ionization energies are for Fe I (7.902 instead of 7.87), YI (6.217 instead of 6.38), and Zr I (6.634 instead of 6.84), all values in eV.

Table 1. Ionization energies for the first through fifth spectra

Element	Z	I	II	III	IV	V
Hydrogen H	1	13.5984				
Helium He	2	24.5874	54.417760			
Lithium Li	3	5.3917	75.6400	122.45429		
Beryllium Be	4	9.3227	18.21114	153.89661	217.71865	
Boron B	5	8.2980	25.1548	37.93064	259.37521	340.22580
Carbon C	6	11.2603	24.3833	47.8878	64.4939	392.087
Nitrogen N	7	14.5341	29.6013	47.44924	77.4735	97.8902
Oxygen O	8	13.6181	35.1211	54.9355	77.41353	113.8990
Fluorine F	9	17.4228	34.9708	62.7084	87.1398	114.2428
Neon Ne	10	21.5646	40.96296	63.45	97.12	126.21
Sodium Na	11	5.1391	47.2864	71.6200	98.91	138.40
Magnesium Mg	12	7.6462	15.03527	80.1437	109.2655	141.27
Aluminum Al	13	5.9858	18.82855	28.44765	119.992	153.825
Silicon Si	14	8.1517	16.34584	33.49302	45.14181	166.767
Phosphorus P	15	10.4867	19.7695	30.2027	51.4439	65.0251
Sulfur S	16	10.3600	23.33788	34.79	47.222	72.5945
Chlorine Cl	17	12.9676	23.8136	39.61	53.4652	67.8
Argon Ar	18	15.7596	27.62965	40.74	59.81	75.02
Potassium K	19	4.3407	31.63	45.806	60.91	82.66
Calcium Ca	20	6.1132	11.87172	50.9131	67.27	84.50
Scandium Sc	21	6.5615	12.79977	24.75666	73.4894	91.65
Titanium Ti	22	6.8281	13.5755	27.4917	43.2672	99.30
Vanadium V	23	6.7462	14.618	29.311	46.709	65.2817
Chromium Cr	24	6.7665	16.4857	30.96	49.16	69.46
Manganese Mn	25	7.4340	15.6400	33.668	51.2	72.4
Iron Fe	26	7.9024	16.1877	30.652	54.8	75.0
Cobalt CO	27	7.8810	17.084	33.50	51.3	79.5
Nickel Ni	28	7.6398	18.16884	35.19	54.9	76.06
Copper Cu	29	7.7264	20.2924	36.841	57.38	79.8
Zinc Zn	30	9.3942	17.96439	39.723	59.4	82.6
Gallium Ga	31	5.9993	20.51514	30.71	64	87
Germanium Ge	32	7.8994	15.93461	34.2241	45.7131	93.5
Arsenic As	33	9.7886	18.5892	28.351	50.13	62.63
Selenium Se	34	9.7524	21.19	30.8204	42.9450	68.3
Bromine Br	35	11.8138	21.591	36.	47.3	59.7
Krypton Kr	36	13.9996	24.35984	36.950	52.5	64.7
Rubidium Rb	37	4.1771	27.2895	40	52.6	71.0
Strontium Sr	38	5.6949	11.0301	42.89	57	71.6
Yttrium Y	39	6.2171	12	20.52	60.597	77.0
Zirconium Zr	40	6.6339	13.1	22.99	34.34	80.348
Niobium Nb	41	6.7589	14.0	25.04	38.3	50.55
Molybdenum Mo	42	7.0924	16.16	27.13	46.4	54.49
Technetium Tc	43	7.28	15.26	29.54	46	55
Ruthenium Ru	44	7.3605	16.76	28.47	50	60
Rhodium Rh	45	7.4589	18.08	31.06	48	65
Palladium Pd	46	8.3369	19.43	32.93	53	62
Silver Ag	47	7.5762	21.47746	34.83	56	68
Cadmium Cd	48	8.9938	16.90831	37.48	59	72
Indium In	49	5.7864	18.8703	28.03	54.4	77
Tin Sn	50	7.3439	14.6322	30.50260	40.73502	72.28

Table 1. Ionization energies for the first through fifth spectra (continued)

Element	<i>Z</i>	<i>I</i>	<i>II</i>	<i>III</i>	<i>IV</i>	<i>V</i>
Antimony Sb	51	8.6084	16.63	25.3	44.2	56
Tellurium Te	52	9.0096	18.6	27.96	37.41	58.75
Iodine I	53	10.4513	19.1313	33	42	66
Xenon Xe	54	12.1298	20.9750	32.1230	46	57
Cesium Cs	55	3.8939	23.15744	35	46	62
Barium Ba	56	5.2117	10.00383	35.84	49	62
Lanthanum La	57	5.5769	11.059	19.1773	49.95	61.6
Cerium Ce	58	5.5387	10.85	20.198	36.758	65.55
Praseodymium Pr	59	5.473	10.55	21.624	38.98	57.53
Neodymium Nd	60	5.5250	10.72	22.1	40.4	60.00
Promethium Pm	61	5.582	10.90	22.3	41.1	61.69
Samarium Sm	62	5.6436	11.07	23.4	41.4	62.66
Europium Eu	63	5.6704	11.25	24.92	42.7	63.23
Gadolinium Gd	64	6.1501	12.09	20.63	44.0	64.76
Terbium Tb	65	5.8638	11.52	21.91	39.79	66.46
Dysprosium Dy	66	5.9389	11.67	22.8	41.47	62.08
Holmium Ho	67	6.0215	11.80	22.84	42.5	63.93
Erbium Er	68	6.1077	11.93	22.74	42.7	65.10
Thulium Tm	69	6.1843	12.05	23.68	42.7	65.42
Ytterbium Yb	70	6.2542	12.176	25.05	43.56	65.58
Lutetium Lu	71	5.4259	13.9	20.9594	45.25	66.8
Hafnium Hf	72	6.8251	15	23.3	33.33	68.38
Tantalum Ta	73	7.5496	16	22	33	45
Tungsten W	74	7.8640	16.1	24	35	48
Rhenium Re	75	7.8335	17	26	38	51
Osmium Os	76	8.4382	17	25	40	54
Iridium Ir	77	8.9670	17	27	39	57
Platinum Pt	78	8.9587	18.563	28	41	55
Gold Au	79	9.2255	20.20	30	44	58
Mercury Hg	80	10.4375	18.7568	34.2	46	61
Thallium Tl	81	6.1082	20.4283	29.83	50.7	64
Lead Pb	82	7.4167	15.03248	31.9373	42.32	68.8
Bismuth Bi	83	7.2856	16.703	25.56	45.3	56.0
Polonium Po	84	8.417?	19	27	38	61
Astatine At	85	9.3	20	29	41	51
Radon Rn	86	10.7485	21	29	44	55
Francium Fr	87	4.0727	22	33	43	59
Radium Ra	88	5.2784	10.14715	34	46	58
Actinium Ac	89	5.17	11.75	20	49	62
Thorium Th	90	6.3067	11.9	20.0	28.8	65
Protactinium	91	5.89				
Uranium U	92	6.1941	10.6			
Neptunium Np	93	6.2657				
Plutonium Pu	94	6.0262	11.2			
Americium Am	95	5.9738				
Curium Cm	96	5.9915				
Berkelium Bk	97	6.1979				
Californium Cf	98	6.2817	11.8			
Einsteinium Es	99	6.42	12.0			
Fermium Fm	100	6.50				

2. Partition Functions

2.1. General Remarks

Abundance codes currently in use employ a variety of algorithms to calculate partition functions. Some of the routines are decades old. The general *method* of calculating a sum over the known states has been known since the early days of quantum mechanics. However, our knowledge of the locations of these states and the computational power to take them into account has changed significantly. Abundance workers would do well to make sure they are using the most complete and accurate material, as well as modern techniques. References to some of the older work on partition functions are given by Gray (1992) and Cowley and Adelman (1983). Other algorithms recently used are those of Traving, Baschek, and Holweger (1966), or Irwin (1981).

2.2. Influence of Completeness on Partition Functions

The degree to which the level structure of a given ion is complete, particularly below about $30\,000\text{ cm}^{-1}$, is critical to the reliability of the partition function for the species. For example, Bord and Cowley (2002) have shown that, at the temperature of the Sun, the partition function for Ho II increases by a factor of nearly 1.5 over that inferred from the 49 published levels (Martin, Zalubas, and Hagan 1978) when contributions from unobserved levels arising from the $(4f^{11}6p + 4f^{10}(5d + 6s)^2)$ group are included. The impact of such changes for stellar abundance work can be quite significant because the number of absorbers scales inversely with the partition function. In the case of holmium in the Sun, raising the partition function by 50% requires an increase in the abundance of this element of 0.17 dex in order to match the strengths of observed lines; this alone is enough to nearly reconcile the photospheric abundance of holmium based on earlier work (Deams, Biéumont, and Grevesse 1984) with that found in CI meteorites.

Cowan (1981, Table 1-4) has assessed the analyses of atomic spectra in his Table 1-4, using a letter scale in which A signifies an essentially complete analysis and F identifies cases where no individual lines are known, only unresolved transition arrays. The Ho II spectrum, for example, is graded C, with only a few dozen or so levels known. Several of the third spectra of the lanthanides were graded C or “worse” by Cowan, leading to the study by Cowley and Barisciano (1994). They used Cowan’s code to complete the level structure of the third spectra of La through Lu for temperatures up to 31,000K. This led to significant revisions of a number of the calculated partition functions at 10,000K (and above). They gave Bolton (1970) coefficients, but the energy levels are available from CRC.

We have recently investigated the completeness of the first and second spectra of the 5d-elements tungsten, rhenium, and osmium for the purpose of re-evaluating the partition functions for these ions. The spectra of all of these species are rated as B (all of the lowest 3 or 4 configurations and portions of some higher ones are known) by Cowan, except for Os II which is graded C.

As features attributable to these ions are increasingly being identified in high resolution, near-ultraviolet spectra of warm stars and used in abundance work (cf. Cowan et al. 2002, Henderson et. al. 1999, Leckrone et al. 1999, and

Wahlgren et al. 1997, 1998), it is worthwhile to re-visit this issue. Inaccuracies in the partition function systematically affect abundances derived from all spectral lines. Thus, as for the ionization potentials, which, for the 5d-elements, are also undergoing revision (see, for example, Campbell-Miller and Simard 1996), care must be taken to use the best available partition functions. In particular, we demonstrate that relying on partition functions based only on the data included in *Atomic Energy Levels, Volume III* (Moore 1958, hereafter AEL), can lead to errors of $\approx 10\%$ or more in some cases for temperatures of 10 000 K and higher. In the following paragraphs, we briefly summarize the status of our investigations.

W I: AEL gives a total of 354 levels, 61 of which are below $30\,000\text{ cm}^{-1}$. Most of the low-lying levels belong to configurations of even parity. Laun and Corliss (1968) re-analyzed the spectrum adding 37 new even levels and 64 new odd levels. Shadmi and Caspi (1969) published a theoretical investigation of the low-lying even levels arising from the $(5d + 6s)^6$ group which provided an interpretation for every level found experimentally below $40\,000\text{ cm}^{-1}$ and predicted the existence of numerous other levels. Based on these predictions, Corliss (1969) was able to identify ten new levels in W I.

We have augmented the AEL data by including all the experimental and theoretical levels below $40\,000\text{ cm}^{-1}$ identified in the above references, and have recomputed the partition function for this ion using this expanded set. At 6000 K, the new partition function, based on 407 levels, is only 1.8% larger than that found using the 354 levels included in AEL. However, at 10 000 K, the difference increases to more than 11%, or about 0.05 dex. Our experience with holmium leads us to expect that the uncertainties in the theoretical energy levels (which are of the order of 100 cm^{-1} or less) do not compromise the accuracy of the resulting partition functions in any significant way.

W II: Ekberg, Kling and Mende (2000; hereafter EKM) have presented an analyses of the low configurations of the second spectrum of tungsten yielding 76 even parity and 187 odd parity levels. Their work adds 13 new levels below $30\,000\text{ cm}^{-1}$ to what is included in AEL, for an increase of about 30% over what is available from this source. At present, the levels below this threshold deriving from the $(5d + 6s)^5$ group are complete. We have up-dated the AEL data by including the new levels from EKM up to $40\,000\text{ cm}^{-1}$ and have re-evaluated the partition function for temperatures in the range 3000 to 34 000 K. At the temperature of the Sun, the differences are small (18.08 based on 137 AEL levels vs. 18.28 based on 173 levels from EKM), and increase only to about 8% at 10 000 K. Although the changes brought about by the availability of the new levels are modest, we urge practitioners to incorporate the EKM results into their analyses.

Re I: Wyart (1978) made a systematic study of the $(5d + 6s)^7$ group in Re I, discovering four new even levels, all lying between $30\,000$ and $40\,000\text{ cm}^{-1}$, and re-interpreting two other levels originally described by Trees (1958). The level structure for this ion is essentially complete below about $30\,000\text{ cm}^{-1}$. Incorporating these small modifications into the AEL data results in essentially no change in the partition function at stellar temperatures for which this ion is likely to contribute meaningfully to the spectrum.

Re II: AEL lists a total of 49 even parity levels for this ion; all are below 40 000 cm^{-1} and most have no term assignments. Only a few contributions from the $5d^56s$ and $5d^46s^2$ configurations are identified, and none from the $5d^6$ are reported. The odd parity levels arising from the $5d^56p$ configuration start at 44 000 cm^{-1} .

We have made preliminary calculations of the placement of the levels from the $(5d + 6s)^6$ group for this ion, and find that as many as 35 (out of a total of 142) should reside below about 30 000 cm^{-1} . This comports well with the 33 even levels given in AEL with energies below this threshold. Thus, we expect that the level structure for this ion is essentially complete below 30 000 cm^{-1} and that the partition function derived from the AEL data should be reliable. We have not, however, recomputed the partition function for this ion using any portion of the high resolution experimental FTS data described by Wahlgren et al. (1997), nor have we tried to compare our Cowan code calculations with the more detailed ones of Henderson et al. (1999).

Os I: Energy levels belonging to the $(5d + 6s)^8$ group for this ion have been classified by Gluck et al. (1964). Forty-six even levels were interpreted, including six that are not in the AEL data; most of the new levels are between 20 000 and 30 000 cm^{-1} . Thirty-two new odd levels were classified, the lowest lying four of which occur between 27 000 and 40 000 cm^{-1} . This work renders the level structure for Os I essentially complete below 30 000 cm^{-1} , but, given the small number of additions to the AEL tabulation, does not substantially change the partition function derived from the AEL data.

Os II: AEL gives 22 even levels, all of which have energies below about 25 000 cm^{-1} . Only five of these have been assigned to the $5d^66s$ configuration. The 17 odd levels identified start at about 37 000 cm^{-1} , and only five are assigned to $5d^66p$. Van Kleef and Klinkenberg (1961) include only four new, high-lying odd levels not present in the AEL tabulation.

We have carried out Cowan code calculations for the $(5d + 6s)^7$ group to better establish the energy level structure for this ion for the purposes of refining the partition function. The calculations have been carried out in the same fashion as was done for holmium (Bord and Cowley 2002), and the computed energies were fitted to the AEL values by the method of least squares. The average deviation between the calculated and experimental energies for the 22 known levels was 72 cm^{-1} (0.3%) over a range of 25 000 cm^{-1} with the best fit atomic parameters.

Using the AEL data, supplemented only by the van Kleef and Klinkenberg results, the 43 known energy levels yield a partition function at 10 000 K of 33.46. At the same temperature, these data augmented by our calculations (for a total of 140 levels) give a partition function of 44.89. This is a 34% increase in the partition function. At the temperature of the Sun (≈ 6000 K), the new partition function is only 12.5% larger. Thus, the addition of the new calculated levels will not alter the solar abundance of osmium by more than 0.05 dex, but it could affect abundance determinations in hotter stars by nearly 0.13 dex.

2.3. The Influence of Levels Above Those Tabulated

It is well known that the partition function for a single atom, isolated in the universe, would diverge if the temperature were finite. It is also known that

this odd situation is irrelevant in the real world, because the sizes of atoms are limited by perturbations from nearby atoms and ions. These perturbations lower the ionization energy and terminate the partition function. Simplistic treatments of the high levels make use of a hydrogenic approximation, and add levels until some cut-off energy is reached. This cut-off is typically equal to the first ionization limit (“the” ionization energies of Table 1) reduced by some amount. Often, only perturbations due to free charges are considered, in which case, the energy reduction is $\alpha Ze^2/\rho_D$, where $Z = 1$ for a neutral atom, etc., ρ_D is the Debye length, and α is a dimensionless constant of order unity.

If the degree of ionization is low, as in the case of cool stars, ridiculously inflated partition functions may result if only Debye fields are considered. If the free electron density is many orders of magnitude lower than the gas pressure, atoms will be ionized by interactions with neutral particles, in which case, the ionization energy is lowered by an amount about equal to $\beta e^2/\bar{r}$, with \bar{r} the mean distance between atoms, and β another constant of order unity.

Halenka (cf. <http://draco.uni.opole.pl/~halenka/>; Halenka and Madej 2002) and his coworkers have considered multiple ionization limits that occur in complex atoms. We refer to their papers, and the book by Griem (1997) for details.

All of these complications may be irrelevant in most cases of interest to those interested primarily in calculating line strengths in stellar spectra. The reason for this fortunate circumstance was pointed out long ago by Van’t Veer-Menneret (1961): *At temperatures where these high levels would become occupied, the atom or ion is mostly ionized to the next stage, and the bloated partition function will cancel from the combined Boltzmann-Saha relations which give the number of atoms capable of absorption.* This provides the basis for focusing on levels below 40,000 cm^{-1} (4.95eV) when computing partition functions for most atoms/ions of importance in cooler stars.

To our knowledge, this comforting situation has not been studied since Van’t Veer-Menneret’s work, and probably should be tested in various relevant portions of parameter space.

3. Sources of Atomic Data

The most convenient sources of atomic data for spectral synthesis are the Kurucz CDROMs and his website (<http://cfaku5.harvard.edu>), and VALD Kupka, et al. 1999, see <http://www.astro.univie.ac.at/~vald/>). A number of more general data bases are available, many linked to one another. Two examples are:

- <http://urania.astro.spbu.ru/staff/afk/AtDatCentre/DtBases/db.html>
- <http://plasma-gate.weizmann.ac.il/DBfAPP.html>.

For individual features (lines, elements), literature searches are facilitated by on-line resources such as the Web of Science and the preprint file on astro-ph:

- <http://isiknowledge.com/>
- <http://xxx.lanl.gov/archive/astro-ph>.

The search engines of common browsers (e.g. google.com) often produce useful material.

We will comment below on some of the url’s which are collected for the reader’s convenience. They lead to codes, and additional references to atomic data. These lists are in no way complete, and there is considerable overlap. As

hardware and organizations change, url's become invalid, and the irritating "url not found" may appear. Often, the relevant material is still available on line but with a different or slightly modified url. Additional surfing efforts may be rewarding.

- <http://physics.nist.gov/PhysRefData/contents.html>
- <http://physics.nist.gov/PhysRefData/Handbook/index.html>
- <http://ccp7.dur.ac.uk/library.html>
- <http://cdsweb.u-strasbg.fr/topbase.html>
- <http://www.astro.lu.se/~hampus/astrophys.html/>
- <http://tlusty.gsfc.nasa.gov/>
- <http://www.umh.ac.be/~astro/dream.shtml>
- <http://verdi.as.utexas.edu/>
- <http://uw.physics.wis.edu/~lawler/>
- <http://star.arm.ac.uk/~csj/Welcome.html>
- <ftp://cdsarc.u-strasbg/cats/J/A+A> (or other journals)
- <http://hebe.as.utexas.edu/at/at.cgi>

Generally speaking, data from the Kurucz or VALD sites will provide the basis for an encouraging synthesis of atomic features in most stars. Details are another matter. Even within small wavelength intervals, of 5 to 10 Å, there are usually a few features for which one cannot find an appropriate atomic line, even by modifying the oscillator strength by an order of magnitude or more. This is typical in a region with molecular features, when using VALD, which had not (as of May 2002) yet included molecules. Steps to change this are in the works.

Anomalously strong or missing lines can also arise from shortcomings of atomic data: Either the lines are not in the data bases, or the oscillator strengths are egregiously in error. We must recognize the difficulty of the task of providing useful oscillator strengths for *all* transitions of possible use in complex spectra such as Fe I. Figure 1 shows a comparison of $\log(gf)$ taken from the Kurucz and VALD sites in the spring of 2002 for wavelengths in the region $\lambda\lambda 4000\text{--}4390$. The VALD values are essentially those from Kurucz (1994), while the K99 values were taken from the Kurucz website (cfaku5, see above) in May of 2002. While the majority of the lines are from theoretical calculations, both lists contain gf -values from NIST compilations (e.g. Fuhr, Martin, and Wiese 1988). These lines would agree perfectly, or very closely, depending on the epoch of the evaluations. All lines arise from classified (accurately known) levels.

The community owes an enormous debt to the compilers and creators of these data bases. The number of people actively working on VALD is very small, while Dr. Kurucz is *personally* responsible for much (if not most!) of the data available in his CDRoms and website. The Kurucz site include standard line-broadening parameters for van der Waals, Stark, and natural broadening. Information for the effects of the atomic nucleus (hyperfine structure, isotope shifts) are also available at his site. The newest file formats will have fields for this information for each wavelength, but at present, most fields have only "placeholder" entries. VALD also lists standard line broadening parameters for each line where available.

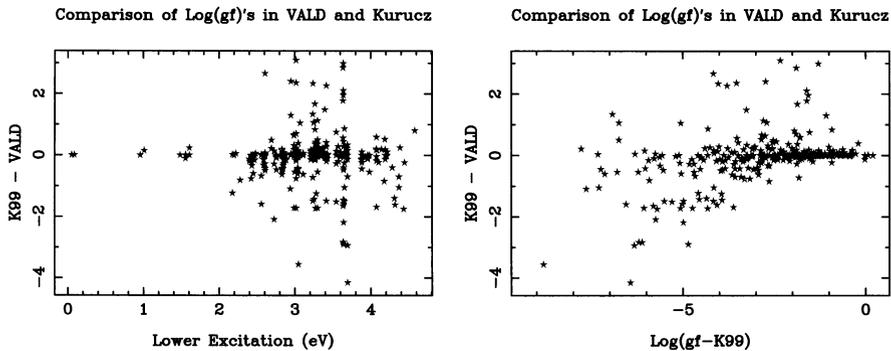


Figure 1. Comparisons of Fe I $\log(gf)$ values in from VALD and the Kurucz site as of May 2002. See text.

It is inevitable that there will be time lags between the availability of new material and its incorporation in the data bases. Having made this clear, it is only prudent to be aware of the shortcomings of this material, both from the point of view of future improvements and making wise use of the data currently available. At present, we favor the Kurucz site for iron and iron-group spectra, and VALD for heavier elements.

It is often helpful to consult recent publications or preprints to obtain atomic data. The url's given at the beginning of this section are useful starting points. Even when data is not given specifically, one may consult references and download PostScript¹ versions. Tables may be converted to ascii text using software such as Ghostscript and Ghostview or similar packages. Many tables in published journals are available in ascii via ftp from the Data Center in Strasbourg (see ftp site above).

4. Photoionization Cross Sections: Implementation of TopBase

While detailed photoionization cross sections have been available from The Opacity Project (cf. Seaton 1987) for more than a decade, the original form was not readily adaptable to synthesis codes. TopBase data files generally consist of several hundred energy levels, corresponding to spectral *terms*, but without the fine-structure splitting. For example, the $^2P_{1/2}$ and $^2P_{3/2}$ of the upper terms of the Na I D-lines are represented by a single energy. Each level may have several hundred to a thousand photon energies, some very closely spaced in order to reproduce “resonances” arising from levels above the first ionization energy. Pronounced lower-frequency structure may arise from such levels that strongly interact with the continuum, photoexcitation of core electrons (PEC), or Cooper minima. Minima also arise because of levels above ionization that interact with the continuum, but which are not connected to the lower level by permitted transitions (cf. Cowan 1981, Fig. 18-6).

¹PostScript is a trademark of Adobe Systems Incorporated

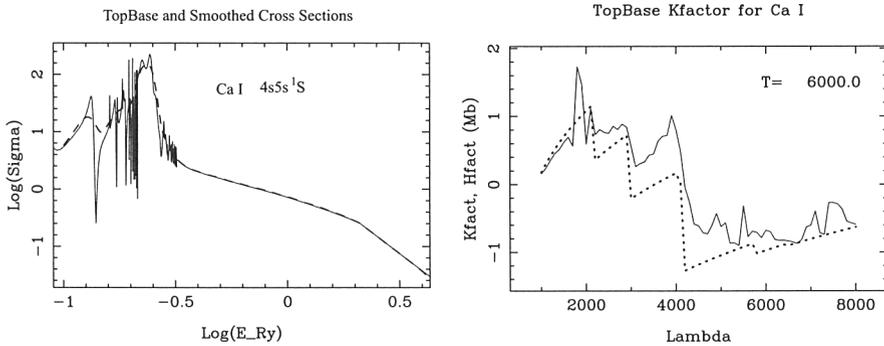


Figure 2. Left: Logarithms of photoionization cross sections vs. energy in Rydbergs TopBase. Fourier smoothed values are shown by the thick dashed line. Right: “K-factors,” or $\Sigma g_n \cdot \exp(-\chi_n/kT) \cdot \sigma_\nu$ vs. wavelength. The sum is over all terms in TopBase for Ca I. The dotted line shows the result if all levels are assumed to have hydrogenic photoionization cross sections. The cross sections in both panels are in Megabarns.

In addition to the sheer complexity of this detail, there has been the practical problem that the sharp resonances in TopBase are included among the Kurucz spectral lines. Moreover, the Kurucz wavelengths are correct, while the TopBase resonances have neither the correct wavelengths nor the proper fine structure. They do have proper Fano profiles and the broad PEC structures, however.

A consensus of TopBase users has emerged, that it is appropriate to smooth over the resonances with a filter that is broader than the sharper resonances, but comparable in breadth to features like the PEC or Cooper minima. Extensive calculations of this type have been carried out (cf. Prieto 2002). An example for one level of Ca I is shown in Fig. 2 (left). The smoothing shown was done by Fourier filtering, but the result is very similar to that obtained by Prieto. Full implementation of the smoothed TopBase cross sections in routines such as ATLAS’s **allop** or **si2op** have yet be completed. These routines give Boltzmann-weighted sums of the cross sections for all levels. Partition functions are not included. The results are shown in Fig. 2 (right) for Ca I. The thick, dashed line shows the corresponding result if hydrogenic approximations are used for each level.

It seems unlikely, however, that future opacity routines will employ algorithms in which atomic levels or terms are treated individually. A more practical approach is to calculate *K-factors*, as defined in the caption above, and to do bilinear interpolation for them in temperature and wavelength. This method is already implemented in routines based, for example, on the calculations of Peach (1970).

5. Molecular Data

The best single site for spectral calculations is probably that of Kurucz, which includes new calculations for TiO and H₂O. We also recommend the following sites:

- <http://www.chem.msu.su/eng/raden>
- <http://cfs-www.harvard.edu/HITRAN/>
- <http://webbook.nist.gov/chemistry/form-ser.html>
- http://diref.uwaterloo.ca/admin_login.html

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