Energy Levels and Observed Spectral Lines of Xenon, Xe I through Xe LIV

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The energy levels and observed spectral lines of the xenon atom, in all stages of ionization for which experimental data are available, have been compiled. Sufficient data were found to generate level and line tables for Xe I–Xe XI, Xe XIX, Xe XXV–Xe XXIX, Xe XLIII–Xe XLV, and Xe LI–Xe LIV. For Xe LIII and Xe LIV theoretical values are compiled for the energy levels. In 15 of the other stages a few lines are reported. Experimental g factors are included for Xe I, Xe II, and Xe III. A value, either experimental, semiempirical, or theoretical, is included for the ionization energy of each ion.
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Key words: compilation; critically evaluated data; energy levels; observed spectral lines; spectra; Xe; xenon; xenon ions.

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1. Introduction

In 1958 Moore [58MOO] published a compilation of the energy levels of xenon containing detailed analyses of Xe I–Xe III and a very partial analysis of Xe IV. In 1968 Striganov and Sventitskii [68STR] published a compilation of xenon lines containing a long list of observed lines for Xe I–Xe III, a limited calculated list for Xe IV, and a few lines for Xe V–Xe VIII. Since these compilations were completed, much work on Xe has been published. This work includes results obtained with new techniques such as laser spectroscopy, beam foil spectroscopy, electron beam ion trap (EBIT), laser excited plasmas, laser implosion, and fusion devices such as tokamaks. As a result we now have energy levels for 24 stages of ionization of Xe and at least one line for 39 stages.

This compilation takes into account published work through December 2002. There are occasional exceptions in which later work is considered, particularly for the ion Xe XI.

Generally, only experimentally derived energy levels are used; these include semiempirical results obtained by interpolation and extrapolation along isoelectronic sequences. An exception is made for Xe LIII and Xe LIV where good theoretical values exist. The use of calculated values is indicated by enclosing the energy value in square brackets for these ions and for a very few levels in other ionization stages.

We tabulate only those lines that have defined levels but include some additional lines in the text for highly ionized stages. For tabulated lines, the wavelengths are compared to the energy level differences and must be consistent to be included. For many of the stages, decisions are made about which of several possible classifications to include by calculating the respective transition probabilities with the Cowan code [81COW]. As a result of this process, in a few cases the line classifications may differ from those given in the stated references.

Occasionally two groups may differ in their published analyses of the spectra of a particular stage of ionization and in the identification of lines belonging to that stage. In such cases we select the analysis we believe to be better. However, the choice is not always clear.

Many laser spectroscopy papers provide data about Rydberg series with results up to very high values of the principal quantum number n. In this compilation we limit the tabulated levels (and thus also the corresponding lines) to include only n less than or equal to 20.

For the first ionization energy we try to provide the best available values obtained experimentally. We do not average experimental values by different authors. Where experimental values are not available, we prefer to use semiempirical results which adjust calculations along an isoelectronic sequence to fit available information about some of the members. For one- and two-electron ions there are very good theoretical values. Where no information of these types is available, we use the calculations of Carlson *et al.* [70CAR] which are based on a simple spherical shell solution for neutral atoms. Their results seem to be within about 7% of valxenon. We note that another calculation was carried out by Magomedov and Omarova [90MAG] using the method of the quasiclassical self-consistent field. The available xenon experimental and semiempirical values tend to fall between the two calculations except for the highest ionization stages.

All energy levels are given in units of cm^{-1} and all wavelengths in units of Å (0.1 nm). Ionization energies are provided in both cm^{-1} and eV. We use the conversion factor $8\,065.544\,77 \pm 0.000\,32\ cm^{-1}/eV$ as determined by Mohr and Taylor [99MOH].

Although it is often difficult to determine, uncertainties in the referenced publication of energy levels and lines are likely 1σ values. In many cases only the number of decimal places indicates the uncertainty in the quoted values. We generally use a ''rule of 20'' whereby an uncertainty of greater than 20 in the least significant digit serves as the criterion for dropping that digit.

The text for each ion does not attempt to provide a complete review of all work on that stage of ionization. Rather, it intends to credit the major contributions, especially those from which values are included in the line and level tables.

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2. Acknowledgments

I wish to thank J. Reader, C. J. Sansonetti, and W. C. Martin for many helpful discussions and advice on the selection of data to include in this compilation. I thank J. Reader for providing prepublication access to the Xe XI data. This work was supported in part by the Office of Fusion Energy Sciences of the U.S. Department of Energy and by the National Aeronautics and Space Administration.

3. Explanation of Tables of Compiled Levels and Lines

In the Energy Level Tables the first column provides the energy level in units of cm^{-1}. The values have been rounded using the ''rule of 20.'' The absence of a decimal point in a whole number is used to indicate that the last digit is not

TABLE 1. Sources of Xe I levels

Source	Number of levels	Method	Adjustment[a] (cm^{-1})	Comment
58MOO	86	Compilation of published and unpublished work to Dec. 1957	$\Lambda-0.508$	To match ground to excited state separation as determined from 01BRA (adjusted)
58THE	20	Classical spectroscopy	$\Lambda-0.508$	To match ground to excited state separation as determined from 01BRA (adjusted)
67HUM	8	Classical spectroscopy	$\Lambda-0.508$	To match ground to excited state separation as determined from 01BRA (adjusted)
70HUM	101	Interferometric spectroscopy on ^{136}Xe	$\Lambda-X$	X given in Table 2. Adjusted to natural isotope mix using several reported isotope measurements and ground to excited state separation as determined from 01BRA (adjusted)
72COD	50	Absorption spectroscopy using synchrotron radiation	None	
81GRA	18	Optogalvanic spectroscopy	$\Lambda-0.508$	To match ground to excited state separation as determined from 01BRA (adjusted)
82LAB	74	Laser excitation with optogalvanic spectroscopy	$\Lambda-0.501$	To match the value we use for the $6p[5/2]_3$ level
85YOS	28	Absorption spectroscopy of discharge source	None	
89HUI	37	Laser spectroscopy	None	
98AHM	16	Optogalvanic spectroscopy	None	Uses same value of reference level as we do to the precision of the results
01BRA	5	Isotope resolved laser spectroscopy	To natural isotope mix	Isotope-specific results adjusted to natural isotope mix by using average weighted by abundance of isotopes in the natural mix

[a]Λ is the value of the level as published. X is given in Table 2.

energy level; "0" signifies even parity and "1" signifies odd parity. The next three columns specify the configuration, term, and J value of the level. In the cases of Xe I–Xe III there is an additional column next which provides the g factor of the level (when known). Finally in the last column a reference is given to the source of the compiled level.

In the Line Tables wavelengths between 2 000 and 20 000 Å are in air. All others are vacuum wavelengths. The first column is the observed wavelength in angstroms (Å). The second column is the vacuum wave number corresponding to the observed wavelength. The wave numbers are provided in units of cm^{-1} for ionization stages Xe I–Xe VI and in units of 10^3 cm^{-1} for the higher ionization stages. The absence of a decimal point indicates that the last zero is not a significant digit. The conversion between air wavelengths and vacuum wavelengths and wave numbers is made using the three-term formula given in Eq. (3) of Peck and Reeder [72PEC]. The wave number values are rounded to the appropriate number of significant digits using the "rule of 20." The third column is the relative intensity assigned to the line. Also included here are codes which are defined for each ion. The next six columns specify the classification of the transition responsible for the line by providing the configuration, term, and J value first for the lower level and then for the upper level. The next to last column is an estimate of the uncertainty in the wavelength of the observed line. The last column identifies the source of the observed line.

Reference

72PEC E. R. Peck and K. Reeder, J. Opt. Soc. Am. **62**, 958 (1972).

4. Tables of Energy Levels and Observed Lines

4.1. Xe I

$Z=54$

Ground state

$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10} 5s^2 5p^6\ {}^1S_0$

Ionization energy 97 833.787±0.012 cm^{-1} (12.129 842 ±0.000 002 eV)

The energy levels of Xe I have been compiled from 11 different sources [58MOO], [58THE], [67HUM], [70HUM], [72COD], [81GRA], [82LAB], [85YOS], [89HUI], [98AHM], [01BRA] which are summarized in Table 1. Where necessary, the published energy levels (denoted by Λ in Table 1) have been adjusted to put all sources on a common basis. The adjustments used are specified in Tables 1 and 2. The largest part of the adjustments has been to obtain a common value for the large separation between the ground state and the excited levels. The value we used was obtained

TABLE 2. Parameter X for adjusting 70HUM levels

Level	X (cm^{-1})
$4f$, $5f-9f$	0.496
$5d$	0.497
$6s$	0.500
$6p$	0.495
$7p$	0.496
$8p$	0.497
$10f$	0.497
all others	0.498

TABLE 3. Sources of Xe I lines

Source	Number of classifications	Light source	Wavelength range (Å)	Uncertainty (Å)
30GRE	2	Geissler tube	5116–5523	0.03 (estimate)
33HUM	410	Geissler tube	3340–10515	0.01 for λ≤9000 Å 0.02 for λ>9000 Å
34MEG	132	Geissler tube (intensities taken from 33HUM)	3948–9923	0.0005 for 4 d.p. lines 0.002 for 3 d.p. lines
35BEU	4	Absorption of carbon arc source	962–996	0.15
35MEG	25	Geissler tube	10 550–12 623	0.03 for 2 d.p. lines 0.1 for 1 d.p. lines
49SIT	5	Flash tube	12 204–19 467	0.5
52HUM	11	Geissler tube	12 451–16 052	0.1
55THE	3	Xe discharges of varying pressures	5963–8559	0.2
58THE	39	Strong Xe discharge at relatively high pressures	3738–10 324	0.2
60HUM	4	Electrodeless discharge tubes	14 355–16 665	Only Ritz wavelengths
61HEP	4	Cooled Geissler tube	23 198–26 518	0.8
63HUM	1	Electrodeless discharge tube	39 210	2.
64AGO	2	Wide band optical maser	32 752	3.
64FAU	3	Maser	34 340–185 140	10.
64PET	1	Electrodeless discharge tube	1470	0.003
67HUM	21	Electrodeless discharge tubes	38 679–40 769	1.
72COD	50	Absorption of synchrotron radiation	430–592	0.02–0.10
72MOR	184	Electrodeless discharge tube	36 518–54 447	1.–4.
73HUM	103	Electrodeless discharge tube	12 409–36 242	Only Ritz wavelengths
85YOS	69	Absorption of He discharge for λ<1070 Å Absorption of Ar discharge for λ>1070 Å	926–1296	0.002 for 3 d.p. lines 0.01 for 2 d.p. lines
98AHM	34	Optogalvanic spectroscopy	6383–6753	0.13
00MIS	24	Electrodeless discharge tube	10 528–21 476	0.003–0.014
01BRA	3	Isotope-resolved laser spectroscopy from ground state	1044–1061	0.000 03

from the isotope-specific results of Brandi *et al.* [01BRA] for the $5p^6-5p^5nl$ energy difference by using an average of values for each isotope weighted according to its fraction in the natural isotope mix. This same method of averaging the isotope-specific values was used to obtain our quoted ionization energy from the isotope specific results of Brandi *et al.* [01BRA].

The first major compilation of Xe I levels, by Moore [58MOO], was largely based on unpublished work of Edlén. Several other sources [58THE], [67HUM], [70HUM], [81GRA] use this work's value for the ground–excited state separation and all are adjusted to the value based on Brandi *et al.* [01BRA]. Several other sources require no adjustment since they measure directly from the ground state [72COD], [85YOS], [89HUI] or, to the precision of their quoted results, use a reference level [98AHM] in agreement with the value used here. The most precise measurement of many excited levels was in the work of Humphreys and Paul [70HUM]. However, their work was for the single isotope ^{136}Xe. In order to be able to use these results, their values were corrected to the natural isotope mix as specified in Tables 1 and 2 by using isotope shift data [89PLI], [74JAC], [75JAC] and a weighted average over the isotopes. This results in a decrease in precision from the four decimal places quoted in Humphreys and Paul [70HUM]. The uncertainty is estimated to be 0.0035 cm^{-1} from the ground state and 0.001 cm^{-1} between excited levels.

Note that in the level table the three energy levels in

[58MOO] by Edlén. The energy of autoionizing levels can be specified in two different ways. One is to specify the resonance energy of the absorption profile. The other is to specify the energy at which the peak of the absorption profile occurs. We chose the latter in order to facilitate the use of these tables with observations of spectra. There is work reported using the former, e.g., [86WAN] and [00KOR].

The observed spectral lines of Xe I have been compiled from 23 distinct sources [30GRE], [33HUM], [34MEG], [35BEU], [35MEG], [49SIT], [52HUM], [55THE], [58THE], [60HUM], [61HEP], [63HUM], [64AGO], [64FAU], [64PET], [67HUM], [72COD], [72MOR], [73HUM], [85YOS], [98AHM], [00MIS], [01BRA] with seven additional sources [32RAS], [36BOY], [55PLY], [56HEP], [61HUM], [67AND], [74TAG] totally superseded by the others. The distinct sources are summarized in Table 3. The priority in our choice of lines which appear in more than one reference is specified as follows by spectral region.

Far ultraviolet (400–1500 Å): [01BRA], [85YOS], [64PET], [36BOY], [72COD], and finally [35BEU].

Near ultraviolet and visible (3000–8000 Å): [34MEG], [33HUM], [55THE] for lines between 5200 and 5710 Å, [30GRE], [32RAS], [58THE], [55THE] outside range specified above, [74TAG], and finally [98AHM].

Near infrared (8000–20 000 Å): [34MEG], [00MIS], [35MEG], [33HUM], [52HUM], [55PLY], [30GRE], [32RAS], [58THE], [55THE], [49SIT], [67AND], [73HUM], [61HUM], and finally [60HUM].

[67HUM], [56HEP], [63HUM], [67AND], [72MOR], [64AGO], [64FAU], [73HUM], [61HUM], and finally [60HUM].

As Table 3 indicates, two sources [60HUM], [73HUM] do not provide observed wavelengths but instead give Ritz wavelengths, which are the wavelengths calculated from known energy levels. Since we do not know the actual wavelengths observed, the Ritz wavelengths are quoted to only one decimal place. The corresponding vacuum wave numbers are also given with only one decimal place. In addition for [73HUM], the values quoted were for the isotope ^{136}Xe. We recalculated these Ritz values to base them on our energy levels for the natural isotope xenon mix and also quoted these to one decimal place.

There are some cases in which the authors' choice of which transition to assign the observed line is questionable. For example, in [73HUM] (using vacuum wavelengths) the 33 536.1 Å line was classified as $5d'[5/2]_2-9p[5/2]_3$. But calculation using the Cowan codes [81COW] indicates that the $6p'[1/2]_1-7d[1/2]_0$ transition should be about 20 times stronger. Its wavelength would be 33 543.3 Å. This may be the line actually observed but we report the classification of [73HUM] here.

The classification of the three electric quadrupole lines is due to Edlén [43EDL]. A few additional lines in the wavelength region 1027–1089 Å have been identified by Abbink [28ABB] as Xe I lines. We have been unable to classify these lines and so have not included them. Where possible we have corrected typographical errors in the references. For example, from the stated energy levels in [85YOS] it was clear that the line reported at 1030.453 Å was really at 1030.435 Å.

The wavelengths of lines between 5200 and 5710 Å given in the unpublished report [55THE] suggested higher precision than those provided by [33HUM]. However, they did not agree as well as [33HUM] with the values predicted by the energy levels. Therefore the results of [33HUM] were given priority over [55THE] resulting in no [55THE] lines in this range being in the Xe I line table.

The large uncertainties in the far infrared wavelengths of [72MOR] (often 4 Å) made classification difficult and multiple classification frequent. Lines and levels included in the tables were limited to $n\leqslant 20$. A few additional lines were reported by [74TAG] but were not included because their ionization stage could not be determined. We also note that some far infrared stimulated emission lines reported by [65LIB] were also not included.

All candidate lines were passed through a program to determine if they correspond to a transition between the known Xe I levels. Only classifiable lines are included in our compilation.

Transition probability calculations using the Cowan codes [81COW] with empirically adjusted configuration average energies were used to help resolve choices between multiple possible classifications of lines. Convergence was not obtained for the 19s, 20s, 20d, and 20f levels and so we could

Intensities have been taken from the stated sources.

The intensity codes given in the Xe I line table are taken from the specified sources. Their meaning is stated below:

Symbol	Definition
a	observed in absorption
h	hazy
hf	line has hyperfine structure
l	unsymmetrical-shaded to longer wavelength
w	wide
E2	electric quadrupole line
f	forbidden line
:	Ritz line from levels in natural isotope mix of xenon. Given to only one decimal place since the observed wavelength was not reported.
—	somewhat less intensity than the value given
*	multiply classified line (two or more classifications of this line share the same intensity)

The g_J values included in the Xe I level table are compiled from eight sources [41GRE], [71CHE], [72PRI], [79HUE], [79HUS$_a$], [79HUS$_b$], [83ABU], [83BIN]. Uncertainties have been included in parentheses for those g_j values for which they were specified.

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