

**Activities of the Data Centers on Atomic Spectroscopy at the
National Institute of Standards and Technology**

W.L. Wiese

| | <u>Director</u> | <u>Workforce</u> |
|---|-----------------|--|
| 1. Atomic Energy Levels and Wavelengths | W.C. Martin | 2 Professionals |
| 2. Atomic Transition Probabilities | W.L. Wiese | 1 ¹ / ₄ Professionals |
| 3. Spectral Line Shapes and Shifts | W.L. Wiese | Occasional Guest Scientists, Contractors |

NIST Data Centers on Atomic Spectroscopy

| | <u>Energy Levels</u> | <u>Wavelengths</u> | <u>Transition Probabilities</u> |
|---|---|------------------------|--|
| Recent Work Areas: (compilations last 2 years) | S, Sc, Cu, Mo | Mg, Sc, Fe | Iron-group elements, selected heavy elements |
| Work in Progress: | OII, Mg, Cr, Co, Ge, Kr | OII, Na, Al, Co, Cu | Be-sequence C-sequence, NI |
| Selected Future Plans: | Volume on H, D, T, He, C, N and O for ORNL "Red Book" series | | |
| | M-Shell elements (Na-Ar), Zw | Na, Al, Si, V, Cr | Selected heavier elements N-sequence O-sequence B-sequence |

In-House Databases at NIST

1. Literature references (Bibliographic database):

All recent literature references (for AEL, since 1985; ATP, since 1980) are entered into a database utilizing ORACLE software and HP 9000 computer. (Assistance by NIST Office of Standard Reference Data in design).

2. Numerical Data:

A general spectroscopic database has been designed by OSRD personnel. Database contains wavelengths, energy levels and transition probabilities in a unified format. Evaluated data on Fe-group elements loaded into database. Again, ORACLE software has been used.

Wavelength Tables and Multiplet Tables Covering Many Elements

- [3] Ultraviolet Multiplet Tables originally issued 1950-1952.
- [12] Multiplet Tables originally issued in 1945.
- [15] Reference Wavelengths, 15 Å to 25000 Å
- [17] Has 39,000 lines of 70 elements, mainly first and second spectra, arranged by element and in a finding list, 2000–9000 Å.
- [27] Has 47,000 lines, first through fifth spectra of all elements, by spectra and in a finding list, all wavelength regions.
- [31] The first part of the tables in [27], with the lines arranged by spectra, were published in the 60th (1979) and later editions of the CRC Handbook. Some corrections have been included in later editions.
- [39] 2000 observed and predicted wavelengths and transition probabilities of magnetic dipole lines for the configurations ns^2np^k , $n=2$ and 3 , $k=1$ to 5 , for beryllium through molybdenum.
- ◆ [48] A compilation of vacuum ultraviolet wavelengths for the elements hydrogen through krypton. Wavelength tables include intensities, upper and lower energy levels, and classifications arranged separately by element and by wavelength.

Wavelength Tables and Multiplet Tables for Particular Elements or a Few Elements

- [1] A critical compilation of energy levels (now superseded by [30]) and multiplet table for Si I.
- [2] A critical compilation of energy levels (now superseded by [30]) and multiplet tables for Si II–IV
- [8] A critical compilation of energy levels and multiplet tables for C I–VI.
- [10, 18] Critical compilations of energy levels and multiplet tables for N I–VII.
- [13] A critical compilation of energy levels and multiplet tables for H I, D, T.
- [19, 23, 25, 29, 35, 51] Critical compilations of energy levels and multiplet tables for O I–VIII.
- [34] A collection of recent spectroscopic data tables for iron; ionization energies, wavelengths, atomic energy levels, and atomic transition probabilities.
- [41] A collection of recent spectroscopic data tables for titanium, chromium, and nickel; ionization energies, wavelengths, atomic energy levels, and atomic transition probabilities.
- [43] A critical compilation of wavelengths, classifications, and intensities for molybdenum ions, Mo VI–XLII.
- [44] A critical compilation of wavelengths, energy levels, level classifications, oscillator strengths, and radiative transition probabilities for nickel ions, Ni IX–XXVIII. Grotrian diagrams are also included.
- [47] A critical compilation of wavelengths, classifications, intensities, and transition probabilities for iron ions, Fe VIII–Fe XXVI.
- [46] A critical compilation of wavelengths and energy level classifications for all scandium spectra.
- [52] A critical compilation of wavelengths, classifications, intensities, and transition probabilities for copper ions, Cu X–Cu XXIX. Grotrian diagrams are also included.
- [53] A critical compilation of wavelengths and energy level classifications for all magnesium spectra.

Bibliographies

- [4, 6, 11, 20, 26, 32, 40] Cover literature since “Atomic Energy Levels”, Vols I–III [9] through December 1987.
Literature since January 1988 are cataloged in the center’s database.

◆Tables published by R. L. Kelly (retired), Naval Postgraduate School, Monterey, CA.

Publications List for Atomic Energy Levels Data Center

1. Moore, C. E., "Selected Tables of Atomic Spectra" (Si II-IV), Natl. Stand. Ref. Data Ser., Natl. Bur. Stand. (U.S.) 3, Sec. 1 (1965). (AEL)
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4. Moore, C. E., "Bibliography on the Analyses of Optical Atomic Spectra", Natl. Bur. Stand. (U.S.), Spec. Publ. 306, Sec. 1 (1968). (AEL)
5. Moore, C. E., and Merrill, P. W., "Partial Grotrian Diagrams of Astrophysical Interest", Natl. Stand. Ref. Data Ser., Natl. Bur. Stand. (U.S.) 23 (1968). (AEL)
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7. Moore, C. E., "Ionization Potentials and Ionization Limits Derived from the Analyses of Optical Spectra", Natl. Stand. Ref. Data Ser., Natl. Bur. Stand. (U.S.) 34 (1970). (AEL)
8. Moore, C. E., "Selected Tables of Atomic Spectra" (C I-VI), Natl. Stand. Ref. Data Ser., Natl. Bur. Stand. (U.S.) 3, Sec. 3 (1970). (AEL)
9. Moore, C. E., "Atomic Energy Levels", Natl. Stand. Ref. Data Ser., Natl. Bur. Stand. (U.S.) 35, Vol. I, Vol. II, and Vol. III (1971). (Reprint of NBS Circ. 467, originally issued in 1949, 1952, and 1958). (NTIS)
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15. Kaufman, V., and Edlen, B., "Reference Wavelengths from Atomic Spectra in the Range 15 Å to 25000 Å", J. Phys. Chem. Ref. Data 3, 825-895 (1974). (ACS)
16. Martin, W. C., Hagan, L., Reader, J., and Sugar, J., "Ground Levels and Ionization Potentials for Lanthanide and Actinide Atoms and Ions", J. Phys. Chem. Ref. Data 3, 771-780 (1974). (ACS)
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33. Martin, W. C., Zalubas, R., and Musgrove, A., "Energy Levels of Phosphorus, P I through P XV," J. Phys. Chem. Ref. Data 14, 751-802 (1985). (ACS)
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50. Martin, W. C., Zalubas, R., and Musgrove, A., "Energy Levels of Chlorine, Cl I through Cl XVII," J. Phys. Chem. Ref. Data, in preparation (1990). (ACS)
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♦Tables published by R. L. Kelly (retired), Naval Postgraduate School, Monterey, CA.

Availability of NIST Publications

Following each publication is a source code symbol in parentheses, e. g., (ACS). This code denotes the availability of each publication and how it may be obtained.

Source Ordering Codes:

- ACS American Chemical Society
 Distribution Office
 Room 210
 1155 Sixteenth Street, N.W.
 Washington, DC 20036
 Telephone: (202) 872-4539
- AEL Atomic Energy Levels Data Center
 National Institute of Standards and Technology
 Physics Building, Room A167
 Gaithersburg, MD 20899
 Telephone: (301) 975-3221
- ALS Data Center on Atomic Line Shapes and Shifts
 National Institute of Standards and Technology
 Physics Building, Room A267
 Gaithersburg, MD 20899
 Telephone: (301) 975-3204
- ATP Data Center on Atomic Transition Probabilities
 National Institute of Standards and Technology
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 Telephone: (301) 975-3204
- CRC CRC Press, Inc.
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- GPO Superintendent of Documents
 U.S. Government Printing Office
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- NTIS National Technical Information Service
 U.S. Department of Commerce
 5285 Port Royal Road
 Springfield, VA 22161
 Telephone: (703) 487-4650
- 0 Out of print--no longer available

Data Centers on Atomic Transition Probabilities and Line Shapes

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Scope: Collects, catalogs, and evaluates data on transition probabilities and oscillator strengths as well as line shape parameters of atoms and atomic ions in the gas phase, as well as radiative lifetimes of atomic and ionic levels. Publishes critical reviews and tables of critically evaluated data, as well as annotated bibliographies. Responds to user requests for data, literature references, and technical information.

References on Critically Evaluated Transition Probabilities

(arranged by spectra)

| | | | |
|---|-------------|--------|------|
| H - Ne | (Z = 1-10) | (1966) | [1] |
| Na - Ca | (Z = 11-20) | (1969) | [2] |
| Sc - Mn | (Z = 21-25) | (1988) | [10] |
| Fe - Ni | (Z = 26-28) | (1988) | [11] |
| Ba I-II | (Z = 56) | (1969) | [3] |
| 63 elements (about 8300 spectral lines) | | (1990) | [9] |

[] The numbers in brackets refer to the publications list numbers on the following pages.

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2. W. L. Wiese, M. W. Smith, and B. M. Miles
"Atomic Transition Probabilities (Na through Ca--A Critical Data Compilation)," Nat. Stand. Ref. Data Ser., Nat. Bur. Stand. (U.S.) 22, Vol. II (U.S. Government Printing Office, Washington, D.C., 1969). (NTIS)

3. B. M. Miles and W. L. Wiese
"Critically Evaluated Transition Probabilities for Ba I and II," Nat. Bur. Stand. (U.S.) Tech. Note 474 (U.S. Government Printing Office, Washington, D.C., 1969); At. Data 1, 1 (1969). (ATP)
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