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COMPUTERIZATION OF ATOMIC LEVEL AND TRANSITION DATA FOR THE FIRST AND SECOND IONIZATION STATES OF THE ELEMENTS HYDROGEN THROUGH PHOSPHOROUS

E. A. Henry

October 6, 1976

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COMPUTERIZATION OF ATOMIC LEVEL AND TRANSITION DATA FOR THE FIRST AND SECOND IONIZATION STATES OF THE ELEMENTS HYDROGEN THROUGH PHOSPHOROUS

Abstract

A computerized data base of atomic energy levels and atomic transition data has been developed from data published by the National Bureau of Standards. These data are of potential use for laser application. The MASTER CONTROL data-base management system is used. These computerized data can be requested from the ERDA Computer Program Exchange and Information Center of the Argonne National Laboratory or from the National Technical Information Service of the U.S. Department of Commerce.

Introduction

Evaluations of atomic energy-level and atomic transition data published by the National Bureau of Standards have been computerized. This data base, ATOM, is managed by the MASTER CONTROL data base management system.¹⁻⁷

Data on the first and second ionization states of the elements hydrogen through phosphorus are included in ATOM. Mass identification is made where this information is available. The scientific annotations and data attributes contained in the printed data evaluations are retained in the computerized version whenever possible.

This work is a continuation of the computerization of scientific data bases at the Lawrence Livermore Laboratory by the Data Management Research Project.^{8,9}

Data Base Contents

Data base ATOM contains both atomic energy-level data and atomic transition data. These two types of data can be used independently of each other though they employ some of the same arrays. The two types of data are distinguished by their record numbers. (See the user interface in the appendix.)

Thirty-two data-base arrays contain the information on eleven basic data items:

1. *ATOM.* This array identifies the atom and ionization state.
2. *IP.* The ionization potential is given.
3. *CONFIG.* The electronic configuration of each level is detailed.
4. *DESIG.* The designation of the term^{10,11} to which the level belongs is given.
5. *LEVEL.* The atomic level energies are given in units of cm^{-1} .
6. *J.* The J-value, the inner quantum number of each level, is given.
7. *LINE* This array gives the intensity of the atomic transitions.
8. *LEVJ, JF* These arrays give the level energy, inner quantum number, and term designation of the atom level at which an atomic transition terminates.
9. *LEVI, JI,* These arrays give the level energy, inner quantum number, and term designation of the atom level at which an atomic transition begins.
10. *INT.* The intensity of the atomic transition is given.
11. *MULT-NC.* The transition multiplet number is identified using the notation of Moore.^{10,12,13}

Each numerical array has a companion array which describes any qualifications of the number. The primary reference information is contained in six reference arrays. Thus the scientific value of the data is retained.

The user interface, UI-ATM, is given in the appendix. It contains comments further details of the data-base structure and array contents.

Availability

Users of the Lawrence Livermore Laboratory computer system may obtain the atomic data base, and the user interface from the IBM-1360 Photostore under the directory .603750:ATOMIC. The data base consists of the index file (ATOM), and five data files (ATOM01, ATOM02, ATOM03, ATOM04, ATOM05), with the user interface (UI-ATM).

Interested users elsewhere may request the data as an energy level data file and a transition data file in a card-image, fixed-field format (see Tables 1 and 2) from:

ERDA Computer Program Exchange and Information Center
 Argonne National Laboratory
 9700 South Cass Avenue
 Argonne, Illinois 60439
 Telephone (312) 739-7711

or

U.S. Department of Commerce
 National Technical Information Service (NTIS)
 5285 Port Royal Road
 Springfield, Virginia 22151
 Telephone (703) 321-8572

Table 1. Card image format for the atomic energy level data.

Card	Columns	Array	Format
1	2-10	IDN	I9
1	11-23	ATOM	A13
1	24-32	IP	F9.5
2	2-30	CONFIG	A29
2	31-54	DESIG	A24
2	55-57	J	F3.1
2	58-59	JN	A2
3	2-13	LEVEL	F12.3
3	14-19	LEVELN	A6
3	20-31	LEVELX	A12
3	32-38	LEVELXN	A7
3	39-68	REMARKX	A30
4	2-71	REMARK	A70
5	2-71	REF1	A70
6	2-71	REF2	A70
7	2-71	REF3	A70

Table 2. Card image format for the atomic transition data.

Card	Columns	Array	Format
1	2-10	IDN	I9
1	11-23	ATOM	A13
1	24-32	IP	F9.5
1	33-43	LINE	F11.4
1	44-48	LINEN	A5
1	49-57	INT	F9.2
1	58-61	INTN	A4
1	62-67	MED	A6
2	2-8	LEVf	F7.4
2	9-12	JF	F4.1
2	13-32	DESf	A20
2	33-39	LEVI	F7.4
2	40-43	JI	F4.1
2	44-63	DESI	A20
3	2-11	MULT-NO	A10
3	12-16	RCODE	A5
3	17-70	REMARK	A54
4	2-71	REF1	A70
5	2-71	REF2	A70
6	2-71	REF3	A70
7	2-71	REF4	A70
8	2-71	REF5	A70
9	2-71	REF6	A70

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12. Charlotte E. Moore, *An Ultraviolet Multiplet Table*, NBS Circular 488, Sect. 1 (1950), Sect. 2 (1952), and Sect. 3-5 (1962).
13. Charlotte E. Moore, *Selected Tables of Atomic Spectra, Atomic Energy Levels, and Multiplet Tables*, NSRDS-NBS 3, Sect. 1 (1965), Sect. 2 (1967), Sect. 3 (1970), Sect 4 (1971), Sect. 5 (1975), and Sect. 6 (1972).

Appendix

User Interface UI-ATM

The user interface UI-ATM outlines the important aspects of data base ATOM.

First, it defines the arrays in which the various data items are contained. These arrays fall into two basic categories: those containing level data and those containing transition data. Certain arrays, such as "ATOM" and "IP," are common to both data categories. Brief descriptions of the contents of each array are given after the array type.

Next, predefined column names and some macro commands are included for convenient output of data using the MASTER CCNTROL program.

Finally, extensive notes are included in the user interface to enable the user to use the data base and interpret the more complex data entries.

The entire user interface is listed in Fig. A1. Figures A2 and A3 display examples of atomic level and atomic transition data contained in the data base. These computer printouts have been created using the column names defined in the user interface.

**** ATOMIC ENERGY LEVELS AND TRANSITIONS ****

```

* REFERENCES:  ATOMIC ENERGY LEVELS BY CHARLOTTE E. MOORE,
*              NBS CIRCULAR 467 VOL. 1 (1949), VOL. 11 (1952), AND
*              VOL. 111 (1958). ALSO REPRINTED AS NSRDS-NBS 35 VOLS. 1,
*              11, AND 111.
*
*              AAN ULTRAVIOLET MULTIPLET TABLES BY CHARLOTTE E. MOORE,
*              NBS CIRCULAR 489 SECT. 1 (1950), SECT. 2 (1952),
*              SECTS. 3-5 (1962).
*
*              ASELECTED TABLES OF ATOMIC SPECTRA, ATOMIC ENERGY LEVELS
*              AND MULTIPLET TABLES BY CHARLOTTE E. MOORE,
*              NSRDS-NBS 3 SECT. 1 (1963), SECT. 2 (1967),
*              SECT. 3 (1970), SECT. 4 (1971), SECT. 5 (1975), AND
*              SECT. 6 (1972).
*
* DATA BASE
* COVERAGE:  THE DATA INCLUDED IN THIS DATA BASE ARE BOTH
*              THE ATOMIC LEVEL DATA BEGINNING WITH RECORD NUMBERS AA221000
*              AND THE ATOMIC TRANSITION DATA BEGINNING WITH RECORD NUMBERS
*              AA221000. SINCE SOME SPECIES HAVE MORE THAN 500 LINES
*              CATALOGUED, THE OVERFLOW IS PUT IN RECORDS BEGINNING WITH
*              AA2251000. DATA ARE CONTAINED FOR THE FIRST AND SECOND
*              IONIZATION STATES OF ELEMENTS HYDROGEN THROUGH PHOSPHORUS.
*
* RECORD
* NUMBERS:  THE RECORD IDENTIFICATION NUMBERS ARE OF THE FORM
*              AAZZ1XXX, WHERE:
*
*              XXX ARE SEQUENTIAL NUMBERS BEGINNING WITH 000 FOR THE
*              GROUND STATE IN ENERGY LEVEL DATA.
*
*              XXX ARE SEQUENTIAL NUMBERS BEGINNING WITH 500 FOR THE
*              LOWEST ENERGY LINE FOR ATOMIC TRANSITION DATA, OR
*              WITH 000 IF 11 12 51 OR 52 (OVERFLOW DATA).
*
*              11 IS THE IONIZATION STATE, 01 FOR THE NEUTRAL ATOM,
*              02 FOR THE ATOM WITH ONE ELECTRON REMOVED, ETC.
*              FOR ATOMS WITH MORE THAN 500 TRANSITION LINES CATALOGUED,
*              OVERFLOW IS PUT IN RECORDS WITH 11 EQUAL TO 51 OR 52.
*
*              22 IS THE ATOMIC NUMBER.
*
*              AA IS THE LAST TWO DIGITS OF THE MASS NUMBER A. AA IS
*              OMITTED IF THE MASS OF THE ATOM IS NOT SPECIFIED.
*              ONLY HYDROGEN AND HELIUM HAVE MASS SPECIFICATIONS
*              IN THEIR RECORD NUMBERS.
*
* UNITS:  THE IONIZATION POTENTIALS ARE IN ELECTRON VOLTS. THE
*          ATOMIC ENERGY LEVELS ARE IN CM-1(-1). THE
*          J-VALUES ARE QUANTUM NUMBERS.
*
* ANNO-
* TATIONS:  ANNOTATIONS FOR EACH ENTRY OR VALUE ARE CONTAINED IN
*           ARRAY 'XXXN' WHERE ARRAY 'XXX' CONTAINS THE ENTRY OR
*           VALUE. THE ANNOTATION ABBREVIATIONS ARE:
*
*           - Q  QUESTIONABLE
*           - PR PREDICTED
*           - EX EXTRAPOLATED
*           - ES ESTIMATED
*           - CA CALCULATED
*           - BR VALUE ENCLOSED IN BRACKETS
*           - UN UNCERTAIN (VALUE FOLLOWED BY '-')
*           - UK UNKNOWN
*           - RU RARE ULTIME
*           - SC DIFFERENT INTENSITY SCALE USED BECAUSE OF A
*              DIFFERENT SOURCE USED OF AUTHOR CITED
*
*           - H  HAZY
*           - B  BLEND
*           - R  SELF-REVERSAL
*           - D  UNRESOLVED DOUBLET
*           - W  WEAK
*
* ADDITIONAL COMMENTS ARE CONTAINED IN THE ARRAYS
* 'REMARKX' AND 'REMARK'. REMARKX CONTAINS INFORMATION
* RELEVANT TO LEVEL ENERGIES GIVEN IN ARRAY 'LEVELX'.
* REMARK CONTAINS OTHER GENERAL COMMENTS.

```

Fig. A1. The listing of UI-ATM, the MASTER CONTROL user interface used with this data base, is reproduced. All *C cards are comments which describe aspects of the data.


```

*
* ARRAYS DEFINED BELOW PERTAIN TO ATOMIC ENERGY LEVELS
*

IDN      1      RECORD IDENTIFICATION NUMBER
ATOM     1      ATOM AND IONIZATION STATE IDENTIFICATION
IP       F      IONIZATION POTENTIAL
CONFIG   1      ELECTRONIC CONFIGURATION
DESIG    1      TERM DESIGNATION
J        F      INNER QUANTUM NUMBER
LEVEL    F      LEVEL ENERGY
LEVELN   1      QUALIFIER FOR ENERGY LEVEL
LEVELX   1      LEVEL ENERGY RELATIVE TO ANOTHER LEVEL, OR UNCERTAIN
              BY A SPECIFIED AMOUNT
LEVELXN   1      QUALIFIER FOR LEVELX
REMARKX   1      INFORMATION ABOUT MEANING OF X IN LEVELX
REMARK    1      GENERAL COMMENTS
JN       1      QUALIFIER FOR J
REF1     1      FIRST PRIMARY REFERENCE
REF2     1      SECOND PRIMARY REFERENCE
REF3     1      THIRD PRIMARY REFERENCE
REF4     1      FOURTH PRIMARY REFERENCE
REF5     1      FIFTH PRIMARY REFERENCE
REF6     1      SIXTH PRIMARY REFERENCE

*
* ARRAYS DEFINED BELOW PERTAIN TO THE ATOMIC TRANSITIONS
*

LINE     F      ATOMIC TRANSITION ENERGY
MED      1      MEDIUM FOR WHICH LINE ENERGY IS GIVEN
LEV1     F      ENERGY OF ATOMIC LEVEL WHICH TRANSITION GOES TO
JF       F      J-VALUE OF LEV1
DES1     1      TERM DESIGNATION OF LEV1
LEV1     F      ENERGY OF ATOMIC LEVEL FROM WHICH TRANSITION STARTS
J1       F      J-VALUE OF LEV1
DES1     1      TERM DESIGNATION OF LEV1
MULT-NO  1      MULTIPLY NUMBER OF TRANSITION
RCODE    1      CODE GIVING PRIMARY REFERENCE FOR THE TRANSITION
LINEN    1      QUALIFIER FOR LINE
INT      F      ATOMIC TRANSITION INTENSITY
INTN     1      QUALIFIER FOR INT
S END

CHANGE KEY
72 S END

DEFINE C-N IDN 19 IDN S END
DEFINE C-N ATOM 13 ATOM AND IDN. S END
DEFINE C-N IP F9.5 ION. POT. S END
DEFINE C-N CONFIG 29 ELECTRON CONFIGURATION S END
DEFINE C-N DESIG 24 TERM DESIGNATION S END
DEFINE C-N J F3.1 J S END
DEFINE C-N JN 2 JN S END
DEFINE C-N LEVEL F12.3 LEVEL ENERGY S END
DEFINE C-N LEVELN 6 LEVELN S END
DEFINE C-N LEVELX 12 LEVEL ENERGY S END
DEFINE C-N LEVELXN 7 LEVELXN S END
DEFINE C-N REMARKX 30 REMARKX S END
DEFINE C-N REMARK 40 REMARK S END
DEFINE C-N REF1 20 REF1 S END
DEFINE C-N REF2 20 REF2 S END
DEFINE C-N REF3 20 REF3 S END
DEFINE C-N REF4 20 REF4 S END
DEFINE C-N REF5 20 REF5 S END
DEFINE C-N REF6 20 REF6 S END
DEFINE C-N LINE F11.4 LINE S END
DEFINE C-N LINEN 3 S LINEN S END
DEFINE C-N LEV1 F7.4 LEV1 S END
DEFINE C-N JF F4.1 JF S END
DEFINE C-N DES1 20 TERM DESIG. (ILEV1) S END
DEFINE C-N LEV1 F7.4 LEV1 S END
DEFINE C-N J1 F4.2 J1 S END
DEFINE C-N DES1 20 TERM DESIG. (ILEV1) S END
DEFINE C-N MULT-NO 10 MULT. NO. S END
DEFINE C-N RCODE 5 RCODE S END
DEFINE C-N INT F9.2 INTENSITY S END
DEFINE C-N INTN 4 INTN S END
DEFINE C-N MED 6 MEDIUM S END

DEFINE MACRO >LEV1: = >LIST HSP C-N ATOM CONFIG DESIG J LEVEL S: S END
DEFINE MACRO >IDN: = >LIST HSP C-N IDN DESIG LEVEL LEVELN S: S END
DEFINE MACRO >J1-L4: = >LIST HSP C-N ATOM CONFIG J LEVEL LEVELN LEVELX
LEVELXN REMARKX S: S END

```

TAPE-DUMP ALL S END

Fig. A1. (continued)

**** ATOMIC ENERGY LEVELS AND TRANSITIONS ****

IDN	ATOM AND ION.	ION. POT.	LEVEL ENERGY	J	ELECTRON CONFIGURATION	TERM DESIGNATION
501000	B-I	0.29600	0.000	0.5	2S(U2) 1U(1)CS.2P	2P(U2)CP(U0)
501001	B-I	0.29600	16.000	1.5	2S(U2) 1U(1)CS.2P	2P(U2)CP(U0)
501002	B-I	0.29600	40040.000	0.5	2S(U2) 1U(1)CS.3S	3S(U2)CS
501003	B-I	0.29600	47857.000	1.5	2S2P(U2)	2P(U2)1U(2)CD
802000	O-II	35.14600	0.000	1.5	2S(U2)2P(U3)	2P(U3)1U(4)CS(U0)
802001	O-II	35.14600	26808.400	2.5	2S(U2)2P(U3)	2P(U3)1U(2)CD(U0)
802002	O-II	35.14600	26829.400	1.5	2S(U2)2P(U3)	2P(U3)1U(2)CD(U0)
802003	O-II	35.14600	40466.900	1.5	2S(U2)2P(U3)	2P(U3)1U(2)CP(U0)
1502000	P-II	19.65000	0.000	0.0	3S(U2)3P(U2)	3P(U2)1U(3)CP
1502001	P-II	19.65000	166.600	1.0	3S(U2)3P(U2)	3P(U2)1U(3)CP
1502002	P-II	19.65000	470.300	2.0	3S(U2)3P(U2)	3P(U2)1U(3)CP
1502003	P-II	19.65000	8882.600	2.0	3S(U2)3P(U2)	3P(U2)1U(1)CD
10101000	H-I	13.59800	0.000	0.5	1S	1S(U2)CS
10101001	H-I	13.59800	82258.913	0.5	2P	2P(U2)CP(U0)
10101002	H-I	13.59800	82258.949	0.5	2S	2S(U2)CS
10101003	H-I	13.59800	82259.279	1.5	2P	2P(U2)CP(U0)

Fig. A2. As an example of atomic level data contained in the data base, 16 atomic levels from selected ions are listed. Column-names defined in the user interface are used for this output.

**** ATOMIC ENERGY LEVELS AND TRANSITIONS ****

IDN	ATOM AND ION. LINE	LEVI	J1	TERM DESIG. (LEVI)	LEV2	J2	TERM DESIG. (LEV2)
301500	Li-I	2741.2040	4.5000	4P(U2)CP(U0)	0.0000	0.5	2S(U2)CS
301501	Li-I	2562.3120	4.8200	3P(U2)CP(U0)	0.0000	0.5	2S(U2)CS
301502	Li-I	2475.0810	4.8900	6P(U2)CP(U0)	0.0000	0.5	2S(U2)CS
301503	Li-I	2425.4280	5.0900	7P(U2)CP(U0)	0.0000	0.5	2S(U2)CS
701500	N-I	5200.2970	2.3800	2P(U3)(U2)CD(U0)	0.0000	1.5	2P(U3)(U4)CS(U0)
701501	N-I	5197.9020	2.3800	1.50 2P(U3)(U2)CD(U0)	0.0000	1.5	2P(U3)(U4)CS(U0)
701502	N-I	3456.4970	3.5800	1.50 2P(U3)(U2)CP(U0)	0.0000	1.5	2P(U3)(U4)CS(U0)
701503	N-I	3456.5434	3.5800	0.50 2P(U3)(U2)CP(U0)	0.0000	1.5	2P(U3)(U4)CS(U0)
1002500	NE-II	460.7250	26.7900	0.50 2P(U6)(U2)CS	0.0000	1.5	2P(U5)(U2)CP(U0)
1002501	NE-II	462.3080	26.7900	0.50 2P(U6)(U2)CS	0.1000	0.5	2P(U5)(U2)CP(U0)
1002502	NE-II	456.3440	27.0500	2.50 3S(U4)CP	0.0000	1.5	2P(U5)(U2)CP(U0)
1002503	NE-II	456.8950	27.1200	1.50 3S(U4)CP	0.1000	0.5	2P(U5)(U2)CP(U0)
1302500	AL-II	2669.1660	4.8200	1.00 3P(U3)CP(U0)	0.0000	0.0	3S(U2)(U1)CS
1302501	AL-II	1670.6100	7.3900	1.00 3P(U1)CP(U0)	0.0000	0.0	3S(U2)(U1)CS
1302502	AL-II	2097.0000	10.5500	2.00 3P(U2)(U1)CD	4.8400	2.0	3P(U3)CP(U0)
1302503	AL-II	2091.5000	10.5500	2.00 3P(U2)(U1)CD	4.8270	1.0	3P(U3)CP(U0)

Fig. A3. This listing of 16 atomic lines shows typical transition data in the data base. The output is created using column names defined in the user interface.