

COMMISSION 14: ATOMIC AND MOLECULAR DATA¹ (*DONNEES ATOMIQUES ET MOLECULAIRES*)

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In recognition of its special interdisciplinary character, IAU Commission 14 is linked directly to the Executive Committee. The Commission's role is to inform the astronomical community of new developments in the diverse fields of research which involve atoms and molecules. Conversely it endeavours to sensitize the research community active in those fields to the specific needs of astronomy, especially concerning basic data and modeling tools. More generally, Commission 14 tries to foster long term relations and collaborations between the two communities and, when necessary, to alert funding authorities to the specific needs of ground and space based astronomy for specific atomic and molecular data.

This report is one of the main contributions of Commission 14 to the information of the astronomical community. Several meetings concerned, at least in part, with the need and availability of atomic and molecular data for astrophysics were also sponsored or co-sponsored. In the last triennium, Commission 14 cosponsored IAU Symposium 194 "Astrochemistry: From Molecular Cloud to Planetary Systems" held in Sogwipo (Korea) from Aug. 23 to 27, 1999 and organized by Commission 34. A Joint Discussion: JD1 on "Atomic and Molecular Data for Astrophysics, New Developments, Case Studies and Future Needs" has been planned for the XXIVth IAU General Assembly in Manchester (Aug. 7-19, 2000) and cosponsored by Commissions 15, 16, 29, 34, 36, 40 and 44. Several other Joint Discussions to be held at the Manchester General Assembly are co-sponsored by this commission.

The present report comprises six sections established by the specialized Working Groups of Commission 14. It is made available on the Commission 14 Website:

<http://ww.obspm.fr/IAU14>

and its mirror <http://cfa-www.harvard.edu/amp/iau14>.

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¹Committee of the Executive Committee.

2. WORKING GROUP 2: ATOMIC TRANSITION PROBABILITIES

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The Data Center on Atomic Transition Probabilities at the National Institute of Standards and Technology (NIST) Gaithersburg, MD 20899, USA is continuing its critical data compilation and bibliographical work. It has contributed all its evaluated transition probability material to a greatly expanded version 2.0 of the NIST atomic spectroscopic database, which has now been installed on the World Wide Web. This database contains about 50,000 transition probabilities with estimated uncertainties and may be accessed via links from the NIST Physics Laboratory WWW homepage at

<http://physics.nist.gov>

Details on this and several other atomic spectroscopy databases on the Internet are given in the report of Working Group 1. The comprehensive NIST bibliographical database, which now contains more than 7000 entries, has been updated through May 1999 and is also available at the above cited World Wide Web site. The current compilation work of the NIST atomic transition probabilities data center is centered on the evaluation and tabulation of numerical data for the lighter elements. Work is in progress on hydrogen, helium, lithium, beryllium, boron, fluorine, neon, sodium, magnesium, aluminum, and silicon. The tabulations include allowed (electric dipole) as well as forbidden (mainly magnetic dipole and electric quadrupole) lines.

Major tabulations of transition probability data during the period 1996 to the present are the following:

(a) The NIST data center published a 532-page volume of critically evaluated transition probabilities for the three elements carbon, nitrogen and oxygen as Monograph No. 7 of the Journal of Physical and Chemical Reference Data [135]. This volume contains about 12,500 transitions for all 21 spectra of these three elements.

(b) A large database for lines starting from the ground states of many atoms and ions has been put on the World Wide Web by the University of Kentucky "Atomic Data for Astrophysics" server (Verner et al.) [130]. Their listings now contain 890,000 spectral lines, and for about 13% of these, transition probabilities are included, which are from the Opacity Project.

(c) A review of neutral atom oscillator strengths, published by Doidge [47], in 1995, has been recently updated [48]. This compendium contains oscillator strengths for atomic resonance lines of 65 elements and has been collected mostly for the needs of laboratory atomic absorption spectroscopy.

(d) Morton [76] has prepared a new compilation containing transition probabilities for resonance lines of heavier elements (Ge-Bi, plus limited data for Tc, Th and U). These data are scheduled to be published in the Astrophysical Journal, Supplement Series, as well as on a website.

The following theoretical and experimental projects have been especially active and have contributed many new numerical data during the last three years:

(a) Large amounts of data have been calculated as part of the Opacity Project and its successor, the Iron Project. In particular, very extensive calculations of transition probabilities for various ions of iron have been undertaken [8, 9, 83, 84].

(b) Raassen and co-workers [102-106, 127] have calculated large quantities of oscillator strengths for ionized atoms of the iron group elements by using the "orthogonal operator" approach. Comparisons with experiments indicate that the results are quite accurate. The data are available on the World Wide Web at

<http://www.wins.uva.nl/research/atom/levels/levtext.html>

(c) Lawler and co-workers [5, 10, 11, 37, 39, 77-79, 88, 132-134] have measured numerous transition probabilities of neutral and singly ionized atoms of the Fe-group as well as of several other heavier elements by a combined branching ratio-lifetime technique.

Finally, it is of interest to note that a number of informative review articles on the status and accuracy of oscillator strength data were given at the 6th International Colloquium on Atomic Spectra and Oscillator Strengths for Astrophysical and Laboratory Plasmas (ASOS 6), the proceedings of which are in preparation (see Wiese and Morton) [136].

The remaining part of this report is a bibliography of selected recent literature references, which contain new transition probability data of astrophysical interest produced during the last three-year period. Thus, this new selected bibliography continues where the last working group report left off. As in the previous reports, the bibliographical material is ordered with respect to element and stage of ionization. Table 1 provides an overview of the bibliographical data by spectrum. The references are identified by a running number, which refers to the general reference list at the end of this report. In the general reference list the literature is ordered alphabetically according to the first author, and each reference contains one or more code letters indicating the method applied by the authors. These code letters are defined as follows:

THEORETICAL METHODS:

Q - quantum mechanical calculations

EXPERIMENTAL METHODS:

E - measurements in emission (arc, hollow cathode, etc.).

A - measurements in absorption (absorption tube, etc.).

L - lifetime measurements (laser induced fluorescence, beam-laser and beam-foil spectroscopy, etc.).

M - miscellaneous experimental methods (for example, Stark effect, astrophysical measurements, etc.).

OTHER:

R - relative values only

F - forbidden transitions (not electric dipole)

CP - data compilations

CM - comments

Table 1. Important Literature References

Ar I: 3,43 Ar II: 6,91,123	Gd I: 75	Pt II: 66
As II: 23	Ge I: 22 Ge II: 23	Rb I: 131
Au II: 69	He I: 51	Re II: 132
B I: 57,62 B II: 54,55,63,68	Hg III: 69	S I: 13,20,25,36,119,122 S II: 82,109,120 S III: 34,121 S VII: 65 S XII: 57
Ba I: 74	K I: 131	Se II: 23
Be I: 55	Kr II: 41	Si II: 80 Si III: 33 Si V: 126 Si VII: 38,64,124 Si IX: 64,124 Si X: 57
Bi I: 24 Bi II: 24,60 Bi III: 24	Li I: 131	
C I: 62,89,139 C II: 57,62,85 C III: 12,46,54,55,85	Lu II: 27	
Ca XV: 2	Mg VIII: 57	
Ce III: 28	Mn III: 127	
Co II: 77,79,93,95,102,105	N I: 108 N II: 29,40,125,128 N III: 57 N IV: 55	Sr II: 31 Ti I: 88 Ti III: 104
Cr I: 37 Cr II: 97	Na I: 131	Tl I: 3,24 Tl II: 59 Tl III: 61
Cu II: 94	Ne I: 117 Ne II: 42,58	Tm I: 5,134 Tm II: 5,100,134
Dy I: 39 Dy II: 39	Ni I: 98,133 Ni II: 52,98,138 Ni XIII: 16 Ni XXIV: 57	V I: 90 V II: 70 V IV: 104
Er III: 137	O I: 32,81 O II: 72,81,86,129 O III: 1,53,81 O IV: 30,57,81 O V: 55,81 O VI: 81 O VII: 81	W I: 113 Xe II: 67,73
Eu III: 110	Os IV: 112 Os V: 7 Os VI: 101	Y III: 31 Yb II: 19
Fe I: 8,10,87,115 Fe II: 10,11,21,49,50,78, 99,103,105,114,116 Fe III: 83,106 Fe IV: 9,56 Fe VII: 35 Fe XI: 15,45 Fe XII: 26 Fe XV: 17,18,44 Fe XXI: 2,92 Fe XXII: 57 Fe XXIV: 84 Fe XXV: 84	P I: 14	Zr II: 118 Zr III: 107
Ga II: 111	Pb I: 24 Pb II: 4 Pd II: 71,96	

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