COMMISION 14: ATOMIC AND MOLECULAR DATA (DONNÉES ATOMIQUES ET MOLÉCULAIRES)

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Introduction

The Commission has, since its inception, been devoted to the continually increasing needs of astronomy and astrophysics for reliable atomic and molecular data a) for diagnostic interpretation of astronomical observations, and b) for support of theoretical modelling of astrophysical situations. At the 1985 Delhi General Assembly, the Commission reviewed the scope of its subject matter, and considered whether it should be extended to include higher energy physical processes than are commonly treated by atomic and molecular data. It was concluded that there was no strong demand for this change, which, if implemented, would make the work of the Commission too diffuse. The appropriateness of the past working group structure was also carefully reviewed in the light of contemporary needs. The following working groups, which have evolved from those of past years, together with their chairmen was approved:

1: Atomic Spectra and Wavelength Standards (excluding primary standards): W.C. Martin
2: Atomic Transition Probabilities: W.L Wiese
3: Collision Processes: A. Dalgarno
4: Line Broadening: N. Feautrier
5: Molecular Structure and Transition Data: W.H. Parkinson

WORKING GROUP 1: ATOMIC SPECTRA AND WAVELENGTH STANDARDS

A. Recent Laboratory Research

Some of the references given at the end of this report are sorted according to spectra in Table 1. A Bibliography on Atomic Energy Levels and Spectra covering the period January 1984 through December 1987 is scheduled for publication in 1988 (76). Since this bibliography includes all atomic spectra for which new data have been published, Table 1 is mainly confined to a selection on the basis of astrophysical interest from work on levels, wavelengths, and line classifications for elements $Z \leqq 30$.

The papers on Fe II and Fe I (Table 1) represent the most recent results of a rather extensive research program being carried out for these important spectra in several laboratories. Additional papers by S. Johansson and collaborators reviewing progress on Fe II and plans for further work are included in (77). The recent extension of the Ti I analysis (39, 40) is also based on new observations over a wide wavelength range. The extension of the V II analysis by Iglesias *et al.* allowed the classification of 149 lines (44).

New accurate wavelengths from laboratory measurements have been published for those lines of Cr I, II (45) and Ni I, II (62) that have also been identified in high-resolution solar spectra over the infrared wavenumber range 9000-1800 cm^{-1}. Biémont and Brault's similar observations of Mg I, II (18) and Al I, II (20) over this same infrared range allowed extensions of the analyses of these spectra. Cooksy *et al.* made precise far-infrared measurements of the ground term $^3P_1$-$^3P_2$ fine-structure intervals in both ^{14}N II and ^{15}N II to facilitate observation of

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these transitions in the interstellar medium (11).

Some of the more extensive additions to data on neutral-atom spectra not already mentioned can be cited here. Ref. (2) includes improved values and accurate series formulas for the energy levels of He I. Eriksson gives new wavelengths for 146 N I lines in the vacuum-ultraviolet region 862-1837 Å (10). Recent data based on absorption observations in the vacuum ultraviolet include the photoionization spectrum of P I from threshold down to 765 Å (24), absorption spectra of S I (840-1220 Å) (26) and Cl I (940-1400 Å) (29), and "subvalence-shell" absorption spectra of K I (400-600 Å) (33) and Zn I (708-760 Å) (72).

B. Compilations of Laboratory Data

Sugar and Corliss have published revised and updated energy-levels compilations for the 235 spectra of the iron-group elements K through Ni (Z = 19-28) in a single volume (78). A compilations of levels for the P spectra was also published (79), and energy-level compilations for the spectra of S (80) and Cu (81) are underway. C.E. Moore's new compilation of levels and multiplets for O III has appeared (82). Adelman _et al._ have prepared a finding list from Moore's multiplet tables for spectra of H, C, N, O, and Si (83).

R.L. Kelly's most recent compilation of atomic lines below 2000 Å has been published (84). These tables, which supersede a similar 1973 compilation, cover all ionization stages of H through Kr in two sections. The first section includes energy-level classifications with observed lines sorted according to spectrum, and the second section is a finding list. Kaufman and Sugar published a compilation of forbidden (magnetic-dipole) lines for spectra of the elements Be through Mo (85). The list includes 406 observed wavelengths and gives predicted wavelengths and transition probabilities for 1660 lines over the range from 100 Å to 25.9 mm. The compilation of spectral data and Grotian diagrams for Ti V-Ti XXII by Mori _et al._ includes observed wavelengths with energy-level classifications (86), as does the similar compilation for Ni IX - Ni XXVIII by Shirai _et al._ (87). Fawcett has published calculations for the most important transition arrays in several isoelectronic sequences and included observed wavelengths in the tables. These include the O I sequence (Mg V - Ni XXI) (88), the F I sequence (Mg IV - Ni XX) (89), the Si I sequence through Ni XV (90), the P I sequence through Ni XIV (91), the S I sequence through Ni XIII (92), and the Cl I sequence (Ar II - Ni XII (93). Biémont's tables for the 3s-3p and 3p-3d transitions for V X through Ni XV (Si I sequence) also include experimental wavelengths (94).

Very complete lists of wavelengths derived from experimental energy levels comprise a part of the output of Kurucz's program of calculations for iron-group spectra (95). This work has been completed for the first and second spectra of the elements Ca through Ni and is being extended to include the first ten spectra of these elements. The accurately predicted wavelengths should allow identifications of weaker lines not yet observed in the laboratory. The data can be obtained from Kurucz in computer readable form.

C. Wavelength Standards

The thorium spectrum emitted from hollow-cathode or electrodeless-lamp discharges is very useful for wavelength calibration of high-resolution spectrometers. Palmer and Engleman's _Atlas of the Thorium Spectrum_ (96) includes an extensive list of lines from 2277 to 13500 Å with wavenumbers accurate to ±0.002 cm^{-1} (±0.0005 Å at 5000 Å). Uranium excited in the above types of discharges also gives a very line-rich spectrum useful for wavelength calibration. The similar atlas for U lists 4928 lines (3848-9084 Å) with wavenumbers accurate to ±0.003

cm^{-1} (97). Sansonetti and Weber have measured a number of the Th and U lines (5750-6920 Å) with uncertainties of ±0.0004 cm^{-1} for Th and ±0.0003 cm^{-1} for U (98). Their measurements show the wavenumber errors of the corresponding lines in the Los Alamos atlases to be well within the quoted uncertainty estimates.

The spectrum of a Pt hollow-cathode discharge with Ne carrier gas will be used for on-board calibration of the High-Resolution Spectrograph for the Hubble Space Telescope. The accurate measurements of this spectrum by Reader *et al.* (99,100) and by Engleman (101) make it an excellent source of calibration wavelengths for spectroscopy over the wavelength range 1100-4100 Å. The completed measurements have yielded some 3200 wavelengths in this range with uncertainties of ±0.0005 to ±0.002 Å (100). Engleman has published accurately measured wavenumbers for about 320 Pt I lines (2200-7360 Å) and also a list of wavenumbers for Pt I lines below 2250 Å as predicted by the reevaluated energy levels (101). A list of some 560 Pt II lines together with accurate Pt II energy levels is also being published (99). A detailed atlas of the Pt hollow cathode spectrum is planned.

Eriksson has published wavelengths for 71 O II lines in the 525-4676 Å range with estimated uncertainties of about 0.001 Å (102). The vacuum-ultraviolet wavelengths (525-835 Å) calculated from the improved energy levels are probably accurate within uncertainties of 0.004 Å at 525 Å to 0.0014 Å at 796 Å. A significant addition to the available calibration wavelengths for the XUV region below 500 Å has resulted from the measurements and analysis of Y VI by Persson and Reader (103). Their complete list of some 900 lines extends from 162 to 2452 Å; the uncertainties of the more accurate Ritz-type calculated wavelengths below 500 Å vary from ±0.0003 to ±0.0020 Å.

Spectral lines of highly-ionized members of the Na I isoelectronic sequence are prominent in some laboratory and astrophysical plasmas, particularly those ionization stages centered around the iron-group elements. Reader *et al.* have critically reviewed and fitted the data for these spectra (Ar VIII - Sn XL) using the best available measurements and their own new observations (104). The fitted wavelengths range from 9 to 713 Å and should be especially useful for calibration in the 50-500 Å region; the uncertainties vary from about ±0.003 to ±0.007 Å.

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TABLE 1

Selected references on energy levels, wavelengths, and line classifications for spectra of elements Z ≦ 30. This table is supplementary to a bibliography in progress (76) and also does not include references described in Sec. B of this report.

He I 1, 2

Be I, II 3

B II 4, 5
B III 5, 6
B IV 5

C IV 7, 8, 9

N I 10
N II 11
N V 7

O I 12
O II 13, 14, 102
O VI 7

F VI 15
F VII 7, 16

Ne VIII 17

Mg I 18, 19
Mg II 18

Al I, II 20
Al XI 21

Si II 22
Si XIV 23

P I 24
P VI-XIII 25

S I 26
SVII-XIV 27
S VIII 28

Cl I 29
Cl IX 30
Co XVI 34, 55

Ni I, II 62
Ni VI, VII 54
Ni XVII 34, 55
Ni XIX 47, 63, 64

Ar III 31
Ar IX 32

K I 33

Ca IX 34
Ca XI 35, 36

Sc V 37
Sc X 34
Sc XII 36, 38

Ti I 39, 40
Ti III, IV 41
Ti XI 34
Ti XIII 36
Ti XIV 42
Ti XXI 43

V II 44
V XII 34
V XIV 36, 38

Cr I, II 45
Cr XIII 34
Cr XV 36, 38, 46, 47

Mn IV 48
Mn XIV 34
Mn XVI 36, 38

Fe I 49, 50
Fe II 49, 51, 52, 53
Fe V, VII 54
Fe XV 34, 55
Fe XVII 47, 56,57
Fe XVIII-XXIV 58
Fe XXIII 59
Fe XXIV 59, 60
Fe XXV 43, 61
Zn I 72
Zn IV 73
Zn XII-XX 74
Zn XIV, XV, XVII 68
Zn XVIII 68, 75
Zn XIX 34

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W.C. Martin
Chairman of the Working Group

WORKING GROUP 2: ATOMIC TRANSITION PROBABILITIES

The Data Center on Atomic Transition Probabilities at the National Bureau of Standards, Gaithersburg, Maryland, 20899, U.S.A. has continued its critical compilation work and maintains an up-to-date bibliographical data base. Work to revise and expand the existing NBS critical data compilations for the allowed and forbidden transitions in Fe-group elements, (Refs. A-D) has been completed. A single volume containing all these data for the Fe-group elements Sc to Ni is in press (Volume III of the NBS series of atomic transition probability tables) and is scheduled to be published in the near future, as a supplement to the Journal of Physical and Chemical Reference Data.

In Table 1 the important recent literature references containing atomic transition probability data are presented, which have been published since the last Working Group report of August 1984; this material is ordered according to element and stage of ionization. For brevity the references are identified there only by the running number of the general reference list given at the end of this report. In order to keep the size of this list within the allowed space, both the spectra listed here as well as the references within each spectrum had to be on a selection basis. However, the NBS Data Center will supply all-inclusive lists of references on specific spectra on request. In the general reference list supplied with this report the literature is ordered alphabetically according to principal authors. Each reference contains one or more code letters indicating the method applied by the author. These code letters are defined as follows: