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WORKING GROUP 4: STRUCTURE OF ATOMIC SPECTRA

A. Recent Laboratory Results and Research in Progress

A Bibliography on Atomic Energy Levels and Spectra covering the period July 1979 through December 1983 is scheduled for publication in late 1984(1). The references in Table 1 are thus limited to papers published or known to be in press in 1984; the selection was made from references giving data on energy levels, wavelengths, and line classifications for spectra of the elements $Z \leq 30$. S. Johansson notes that the spectra under investigation in the Physics Department of Lund University, Sweden, include S III, IV, VII, VIII, IX; Cl VI, VII, VIII, X; Sc V; the (Ne I) isoelectronic spectra Sc XII-Fe XVII; Ti I; Cr I, II, V; Fe II, III; and several high-ionization spectra of Ni, the work on Fe III and the Ni spectra being done in collaboration with researchers in the Zeeman Laboratory, Amsterdam. Term analyses in progress at the Lund Institute of Technology, as reported by W. Persson, include Ne III and K II, III. This group has recently completed analyses for Kr IV, Rb V, Sr V, VI and has papers in preparation for Rb IV, Y VI, and Xe II. Fourier-transform spectrometric observations at the National Solar Observatory (Kitt Peak) by J. Brault and collaborators are yielding more accurate and complete line lists for the first and second spectra of several elements, including Mg, Al, Ti, V, Cr, Fe, and Ni. Ongoing extensions of the term analyses for some of these spectra were mentioned above; similar work is underway for Mg I, II, Al I, II, and V I, II (E. Biémont, University of Liège) and for Fe I (R. C. M. Learner, Imperial College, London). B. C. Fawcett's current research at the Rutherford Appleton Laboratory, Oxfordshire, England, includes work on the oxygen-like spectra P VIII through Fe XIX.

B. Compilations, Isoelectronic-Sequence Observations and Predictions

The NBS Atomic Energy Levels Data Center published energy-levels compilations for all the spectra of Fe(29) and Si(30). Revised and updated energy-levels compilations for the 235 spectra of the ten iron-group elements K through Ni will appear in a single volume in 1985⁽³¹⁾. A compilation of levels for the P spectra has also been submitted⁽³²⁾, and C. E. Moore has prepared new tables of levels and multiplets for O IV and O III⁽³³⁾.

R. L. Kelly's revised compilation of atomic lines below 2000 Å is scheduled for publication in 1985⁽³⁴⁾. These tables supersede a similar 1973 compilation and cover the same elements, H through Kr. Fawcett's review⁽²⁸⁾ includes tables of observed forbidden lines for ions stripped to the $n=2$ and $n=3$ shells. Some of the tables of atomic wavelengths in the CRC Handbook were revised and updated for the latest edition⁽³⁵⁾; about 45000 lines from the first five spectra of all elements in all wavelength ranges are included.

A number of papers give energy levels and/or wavelengths as observed or predicted along isoelectronic sequences. Some of the predictions are sufficiently accurate to be used for line identifications in high-ionization spectra. Peacock et al.(15) have measured wavelengths of lines of Ar, Ti, Cr, Fe and Ni in ionization stages belonging to the Li, O, F, Na, or Mg isoelectronic sequences; for the F-like and Mg-like ions, predicted wavelengths are listed for the elements to Mo ($Z=42$). B. Edlén has further refined his methods to obtain accurate predictions for the $n=2$ configurations of the Li, Be, O, and F sequences(36), the B sequence(37), the N sequence(38), and the C sequence(39). These papers include critical compilations of pertinent experimental results, as does Edlén's survey of magnetic-dipole lines in the spectra of ions of the elements Cr to Ag(40). Fawcett's tabulations of calculated quantities for the Be(41), F(42), Mg(43), and Al(44) isoelectronic sequences include predicted wavelengths and, in most cases, experimental wavelengths for some transitions. Recent calculations by Hata and Grant(45) give predicted wavelengths for selected lines of He-like, Li-like, and Be-like ions of the elements Ca to Cu. Additional references for isoelectronic-sequence predictions are given in(1) and in the report of Working Group 2.

TABLE I

Selected references on energy levels, wavelengths, and line classifications for spectra of elements $Z \leq 30$. This table is supplementary to a recent bibliography (1) and also does not include references described in Sec. II of this report.

Fe VII (2)	V II (17)
	V XIV (14)
Mg I (3)	
	Cr XV (14)
Al I (3)	Cr XX, XXI (18)
Al IV (4)	Cr XXII, XXIII (19)
Al VIII-X (5)	
Al XI (6)	Fe II (20)
	Fe XV (21)
Si I (7,8)	Fe XVII (14,22)
	Fe XVIII-XX (15)
S I (9)	
S III (10)	Co III (23)
S VII (11)	
	Ni XIX (14,22)
Cl VII (12)	
	Cu XXVI-XXVIII (24)
Ar IX (13)	
	Zn IV (25)
Sc XII (14)	Zn VI (26)
	Zn XIV-XIX (27)
Ti XIII (14)	
Ti XIV-XX (15)	
Ti XXI, XXII (16)	

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W.C. Martin
Chairman of the Working Group

WORKING GROUP 5: MOLECULAR SPECTROSCOPY

A. Compendia. Bibliographies. Atlases

Research in molecular spectroscopy over much of the electromagnetic spectrum has continued intensively over the past three years. It has been stimulated not only by the imperatives of fundamental research programmes in many laboratories, but also by the impact of molecular lasers on the field, and the needs of atmospheric and environmental programmes. The literature is so prolific that it is impossible even to review briefly here all that is relevant to astrophysical needs. Thus most of this report has been compiled from the contributions from individual workers and Research Centres.

The bi-monthly Berkeley Newsletter(1) compiled from molecular spectroscopic publications in more than 30 journals continues to be a prime bibliographic tool for its more than 500 subscribers.

B. Molecular Data

1. ELECTRONIC BAND ANALYSES AND CONSTANTS OF DIATOMIC MOLECULES

Using laser spectroscopic methods Linton et al.(2) in a collaboration of workers from four laboratories, have continued their definitive studies of the CeO spectrum. The energies of 16 low lying states have been determined and quantum numbers assigned with certainty to 14 of them, and identification and analysis tables are provided for many bands.

Hirota and collaborators at the Institute of Molecular Science at Okazaki have an extensive programme on the microwave and infrared spectra of CH₃(3,4), HO₂(5), SiN(6), PO(7,8), HCCN(9) and FeO(10). Hefferlin(11) continues his theoretical and numerical studies on the systematic properties of constants of diatomic molecules.

2. TRANSITION PROBABILITIES, LIFETIMES, INTENSITIES

Dressler (Zurich) reports the following experimental and theoretical studies on f- values, lifetimes, and transition moments for band systems of NO, N₂ and H₂. Experimental and theoretical studies have been made on transitions between excited ²II states of NO by Gallusser and Dressler(12). Similar work has been done for transitions between singlet states of N₂ by Stahel, Leoni and Dressler(13). An extensive study of lifetimes and transitions probabilities for a number of H₂ states and transitions between them are also reported(14-18).

Sharp (Munich)(19) has developed an efficient computational method for numerical evaluation of Morse Franck-Condon factors and r-centroids of molecular band systems.