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M. J. SEATON

Chairman of the Committee

COMMITTEE 4: STRUCTURE OF ATOMIC SPECTRA

General work on Atomic Spectra

A current *Bibliography on The Analyses of Optical Atomic Spectra* is in print (43). It appears in four sections, three of which cover the same elements as the respective volumes on *Atomic Energy Levels*. Relevant literature references from the dates of publication of these Volumes are continued for each spectrum to the present, as follows:

- Section 1 $^1\text{H} - ^{23}\text{V}$ issued September 1968.
- Section 2 $^{24}\text{Cr} - ^{41}\text{Nb}$ issued February 1969.
- Section 3 $\left\{ \begin{array}{l} ^{42}\text{Mo} - ^{57}\text{La} \\ ^{72}\text{Hf} - ^{89}\text{Ac} \end{array} \right\}$ issued May 1969.

The last Section contains references to rare-earth spectra:

- Section 4 $\left\{ \begin{array}{l} ^{57}\text{La} - ^{71}\text{Lu} \\ ^{89}\text{Ac} - ^{99}\text{Es} \end{array} \right\}$ issued September 1969.

The present report will be limited to later work.

Monographs, extended analyses, work in progress

The active programs in Lund are providing data on atomic spectra that are urgently needed. In the Physics Department of the University, Edlén and his colleagues have published or submitted

for publication analyses on the following spectra:

BeI, BeII (30); BIII (46); FI (49), FII (48); AlI (20).

Analyses are nearly completed or ready for publication for BII (47); Cv (35); NI (21); TIII, TIV (59). Comprehensive work is in progress on OII (61) and on FIII, FIV, FV (50). Edlén has also reported his progress on the complex spectrum Ferv (16), which is one of the most important contributions to astrophysics.

At the Lund Institute of Technology Minnhagen and his associates have investigated CaIII (5) and are working on NeII (51), KII (41), and MgIII (2). Bockasten and associates at Lund and Uppsala have published work on Ov (4a) and OIV (7).

In Madrid at the Institute of Optics the analysis of VIII is in course of preparation (33) and the analyses of VII (60), MIII (24) and NIV (25) have been published. For NiIV, see, also (52).

At the National Bureau of Standards the analyses of ClI (53), ZnII (38) and TcI (6) have been extended.

At the Corona Laboratory Humphreys (32) has recalculated the values of selected energy levels for $^{86}\text{KrII}$ and $^{136}\text{XeII}$ derived from new interferometric observations in the 4μ region.

Vacuum UV atomic spectra

In the HeI sequence lines in the spectra ArXVII through ZnXXX have been observed by Cohen and his associates in the range $4\text{--}1.4\text{ \AA}$ (11). Gabriel and Jordan have reported observations of long wave satellites to the resonance lines of He-like ions in both the laboratory and the Sun; they list laboratory wavelengths for the spectra C through Al (23).

New classifications have also been made in the spectra of the iron-period elements of the ArI, ClI, and SiI sequences by Fawcett *et al.* (22). These authors have studied the configurations $3s^2 3p^n\text{--}3s^2 3p^{n-1}4$, $5s$, 4 , $5d$, in the far vacuum UV region.

Lines of OVI have been observed in emission near 150 \AA with a laser-produced plasma as source (8).

Blake and House (4) have reported observations of K α X-ray-type transitions $1s^2 2s^2 2p^{n-1}\text{--}1s 2s^2 2p^n$ in the solar atmosphere and in laboratory plasmas for: NeIII, SiVII, CrXVIII, FeXX.

M. Chaghtai has observed and analyzed the spectra: ZrV, ZrVI, ZrVII; NbVI, NbVII, NbVIII; MoVII, MoVIII, MoIX (9). This work has been carried on at the Lab. de Chimie physique, Orsay and also in Lund.

Garton and his associates have continued their valuable program on the observation of absorption series: BeI (26), $2s np (n \sim 20)$; Ca, Sr, Ba $< 500\text{ \AA}$, inner shell excitation (28); SrI Singlets of Principal Series to $n = 33$ (27); CsI, RbI (13).

New absorption series and ionization potentials have been reported by Huffman *et al.* (31) for OI and for FI, Bri, ClI, II in the range $600\text{--}1500\text{ \AA}$.

Autoionization is a subject that becomes increasingly important as observational techniques develop. In Ne, autoionizing levels have been determined from observations of 13 absorption series observed by ion impact (19). Madden and his staff have observed resonances in the photo-ionization continuum of ArI ($20\text{--}150\text{eV}$) (37).

Edlén has extended his identifications of the coronal lines by a study of the transitions from metastable levels in the configurations $3s^2 3p^k 3d$ with $k = 3, 4, 5$ of FeXI, FeX, FeIX, and NiXIII, NiXII, and NiXI (17). These transitions "can well account for all of the remaining unidentified coronal lines". In the same paper he confirms the identification of $\lambda 4412$ as ArXIV and of $\lambda 5533.4$ as ArX, by a study of the Z-dependence of the 2p intervals of the configurations $2s^2 2p$ and $2s^2 2p^5$. Edlén *et al.* have also published a paper entitled 'Spin-Forbidden Resonance Multiplets in Light Elements' (18).

A number of theoretical papers deal with highly-ionized spectra. In the HeI isoelectronic sequence analytical wave functions have been calculated up to NVI for the $1s np^{1,3}P$ states for $n = 2, 3, 4, 5$ (1). Eigenvalues and orbital wave functions have been calculated for the 1S states, $n = 1\text{--}3$ and for the 3S states, $n = 2\text{--}4$ for HeI, LiII and BeIII (12). Close-coupling calculations of the positions and

widths of the lowest-lying autoionizing D states in He converging on the $n=2$ level of HeII, have also been made (14).

In the BI isoelectronic sequence Lexa (34) has determined by extrapolation the 12 lowest levels in the spectra SXII through CaXVI.

Hartree-Fock Wave Functions have been calculated for the highly-ionized spectra FeXXII, FeXXIII, FeXXIV, FeXXV (10).

Rare-earth spectra

At the National Bureau of Standards, active work on rare-earth spectra of the lanthanides is being emphasized in order to provide data for Volume IV of *Atomic Energy Levels*. The spectra being investigated are: CeI; PrI, PrIII (58); PmI, PmII; HoI; TmI, TmII, TmIII; YbI and in addition LaIV and ThI. A brief summary has been published (44).

With the aid of Zeeman observations, Blaise and Van Kleef have extended the analyses of GdII (3). Infrared observations of Gd have been reported by Spector and Held (57).

Theoretical work on rare-earth spectra is being continued at the Hebrew University in Israel by Z. B. Goldschmidt and others. In a paper on 'Magnetic Interactions in Heavy Atoms' the authors discuss the $4f^N$ configurations in PrIII, PrIV and ErIV, as well as the $3d^N$ configurations in third spectra of the iron group (29).

Theory and miscellaneous

A number of theoretical papers should be cited. Lotz has calculated 'Subshell Binding Energies of Atoms and Ions, H to Zn' (36), giving preference to experimental values in all doubtful cases. Czyzak and others have calculated collision strengths for the NiI($2p^3$), OI($2p^4$), SiI($3p^2$) and SiI($3p^4$) isoelectronic sequences in a paper on 'Excitation of Forbidden Lines' (15). Minnhagen and Svensson have calculated the energy level distributions and eigenvectors for the $3p^4 nf$ configurations of ArII (42). R. D. Cowan is working on *ab initio* theoretical calculations of atomic energy levels and transition probabilities, primarily in the $p^m l$ configurations of ions isoelectronic with the third-row elements (Na-Ar). Shadmi and his associates have calculated levels and g -values in the second and third spectra of the iron group taking into account effective interactions between d -electrons (55, 55a). They have also made a theoretical study of the even levels in W I (54). C. Roth has made extensive theoretical calculations of levels and g -values for odd configurations in the first, second and third spectra of the iron group, by fitting parameters to the observed data (53a). The odd configurations of TiI have been interpreted theoretically by Smith and Siddall (56). *Ab initio* calculations of the odd configurations of CdI have been reported by Wilson (62).

Martin and Sugar at the National Bureau of Standards have published a paper on 'Perturbations and Coupling in the $d^9 sp$ configurations of CuI, ZnII, AgI, CdII and TlIII' (39). One on the calculations of the $d^9 ns$ configurations in ZnII and AgI, which contains some new levels in these spectra (40) has, also, been published by Martin and Kaufman.

In response to a steady demand for a revised table of ionization potentials, such a compilation is now in course of preparation (45). It is planned to include for each spectrum not only the ionization potential in eV, but also the limit in cm^{-1} used in the calculation. In addition, the energy levels from the ground configuration, above the ground state zero, will be tabulated. References to the source material used for the various spectra will be included.

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CH. MOORE-SITTERLY
 Chairman of the Committee

COMMITTEE 5: MOLECULAR SPECTRA

The laboratory study of molecules of interest to astrophysicists has been progressing at a steady pace. A complete bibliography for the year September 1968 to September 1969, for instance, would show work on 68 molecules of possible interest; the diatomic and simpler polyatomic molecules. During this period 38 papers appeared on H_2 alone, notably on its polarizability and the character of its spectrum near the ionization limit. Twenty-one papers on CO included studies in the vacuum UV, its Franck-Condon factors, chemiluminescence and IR absorptances. In the interests of saving space in this report, the detailed discussion of published work on each molecule of interest will be deleted. Instead, attention might be called to the fact that a complete card file bibliography is maintained by Phillips at Berkeley, and inquiries are welcome. In addition, a bi-monthly *Newsletter* is distributed from Berkeley in collaboration with S. P. Davis of the Physics Department. This *Newsletter* includes information on work currently in progress at various laboratories. At the present time it is being distributed to over 250 spectroscopists in various countries. A further source of information is a bibliography of articles on 'Spectroscopy of Interest to High Temperature Chemistry', which is distributed at frequent intervals by Leo Brewer in the Chemistry Department at Berkeley. Of more limited scope are the annual *Technical Reports* of the Laboratory of Molecular Structure and Spectra of the University of Chicago, which is a collection of their papers. A bibliography of similar scope is distributed periodically by the Joint Institute for Laboratory Astrophysics at Boulder, Colo. Finally, a quite complete bibliography is to be found in *Current Papers in Physics*, published twice monthly by The Institution of Electrical Engineers, Savoy Place, London W.C.2.

Two papers from the National Research Council of Canada should be mentioned, since they are of special astrophysical interest. These are the paper by the late P. G. Wilkinson on H_2 (*Can. J. Phys.*, **46**, 1968, 1225) and one by S. K. Luke on H_2^+ (*Astrophys. J.*, **156**, 1969, 761). The first gives the precise wavelengths of the UV H_2 lines, which will surely be observed in interstellar absorption in the near future, and the second gives the expected radio spectrum of H_2^+ , which may also be observed sooner or later.

In addition to work in progress at various laboratories reported in the *Newsletters*, G. Herzberg has submitted the following for inclusion in this Report:

One of the most interesting results at NRC has been the recent observation by J. W. C. Johns of a spectrum of ArH corresponding to transitions between two Rydberg states of this molecule. The work on CH reported on in previous IAU reports is now in press (G. Herzberg and J. W. C. Johns). An extension of the spectrum of SiH in the vacuum UV has been completed (G. Herzberg, A. Lagerqvist, B. J. McKenzie, *Can. J. Phys.*, in press).

G. Herzberg has carried out a good deal of work on the absorption spectrum of molecular hydrogen (including HD and D_2) in the region below 900 Å. The discrepancy between the theoretical and experimental value for the dissociation energy of hydrogen has been resolved in favor of the theoretical value. The previous experimental values by Monfils and Herzberg were severely affected by lack of resolution and overlapping lines. The new experimental values are based on spectra taken