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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

at liquid nitrogen temperature with the 10·5 m vacuum spectrograph. In addition the Rydberg series of H_2 and its isotopes are being studied.

Following the work on a new spectrum associated with C_2 in the visible region (G. Herzberg and A. Lagerqvist, *Can. J. Phys.*, **46**, 1968, 2363) Milligan and Jacox at NBS by means of matrix work at liquid helium temperature have confirmed the NRC suggestion that this spectrum is due to C_2^-. Three new electronic transitions of C_2 have been observed in the vacuum UV by A. Lagerqvist, C. Malmberg, and G. Herzberg (*Can. J. Phys.*, **47**, 1969, 2735). These spectra may be of interest when far UV spectra of carbon stars become available.

Dr. Ch. Jungen, now of NRC, in collaboration with E. Miescher, has produced a very convincing analysis of the *f* complex of the NO molecule based on high resolution plates in the vacuum UV taken at NRC.

Venkateswarlu, also using the 10·5 m vacuum spectrograph at NRC, has obtained and analysed very extensive spectra of Br_2 and I_2 in the vacuum UV.

B. L. Lutz and A. E. Douglas at NRC have submitted a short paper in the *Canadian Journal of Physics* on the observation, for the first time, of the spectrum of SiH^+. A $'\pi-'\Sigma$ band system, analogous to the CH^+ system, has been found with its 0–0 band origin at 25025·20 cm^{-1}. This band system may give discrete interstellar absorption lines at 3993·400 Å [R(O), 0–0 band] and 3932·347 Å [R(O), 1–0 band] and also the system may occur in the solar spectrum.

Aert Schadee (*JQSRT*, **7**, 1967, 169) has stressed that an electronic *f*-value for molecular transitions is not uniquely defined, but that a wavelength dependent $f_{el}(\lambda)$, multiplied with the Franck-Condon factor, is a fair approximation of the band oscillator strength $f_{v'v''}$ for the stronger bands of a system. He also discusses the normalization of Hönl-London factors in connection with the relation between individual line and band oscillator strengths.

The Berkeley analyses of molecular spectra have resulted in the publication by the University of California Press of Volume 2 comprising analyses of 36 bands of the C_2 Swan system. Also included in this volume is the analysis of the HgH spectrum, which is of less astrophysical interest. Volume 3 on the spectrum of TiO should be ready for publication before the end of 1970. At present in the region 4000–9000 Å TiO analyses are complete for (a) 12 bands of the α-system, (b) 4 bands of the β-system, (c) one band of the γ'-system, (d) 17 bands of the γ-system, (e) one band of the δ-system. Work is continuing on further TiO bands in this same spectral region, and attempts are being made to extend the observations farther into the photographic IR.

Nicholls has been continuing the publication of his very useful series of identification atlases of molecular spectra. In addition to the three atlases referred to in our previous report, he and his co-workers have published (a) the O_2 ($\beta^3\Sigma_u^- - X^3\Sigma_g^-$) Schumann-Runge system, and (b) the C_2 ($A^3\pi_g - X'^3\pi_u$) Swan system.

Recent extensions of astronomical observational capabilities into the UV and IR have created demands for laboratory data that are, at the present time, unavailable. Some of these needs are listed below, in the hope that, by calling attention to them, they will stimulate further laboratory work in these directions.

As an aid in the study of the IR spectra of late-type stars, Spinrad and Wing have called attention to the need of analysis of the IR system of VO. Furthermore, more laboratory work is needed on the diffuse bands of VO between 9530 Å and 9590 Å that were found by Lagerqvist and Selin to accompany the 1·06 μ bands in their laboratory emission spectrograms.

A higher resolution laboratory study is needed of the first overtone sequence of CH rotation-vibration bands in the 2·0–2·3 μ region.

The CN Red System should be observed with high resolution in the IR, notably the $\Delta v = -1$ and $\Delta v = -2$ sequences. The recent improvement of the rotational and vibrational constants of this sytem by Fay, Marenin and Van Citters (*Astrophys. J.*, in press) makes possible improved predictions of line locations in the IR, but even these predictions become uncertain for higher *J*.

Infrared ZrO bands are known that have not yet been classified. Afaf has suggested an analysis involving a system of five-headed bands, indicating that the system involves either triplet or quintet levels.

A feature attributed to HF has been seen at 2·3 μ in the spectrum of α Ori. Data on the molecular equilibrium are lacking.

The polyatomic molecules HCN and C_2H_2 are being considered more and more frequently in connection with absorption features in stellar spectra in the 2 and 3·1 μ regions. Such studies are hampered by lack of measures of these band profiles and intensities for lines with $J > 30$.

In the case of late-type stars, Vardya has called attention to the importance of certain negative molecular ions, notably OH^-, C^-, CN^-, SH^-, H_2O^-. The corresponding rotational and vibrational constants are largely unknown. Furthermore, the electron affinity of HS, C_2 and CN are quite uncertain. Various values in the literature differ by as much as 1 eV. The absorption X-sections for none of these ions are yet available.

Methane and ammonia are important in the spectrum of Jupiter, however, one still lacks data on the absorption profiles of these molecules at the temperatures, pressures and concentrations encountered in Jupiter. For instance, Gillett, Low, and Stein (*Astrophys. J.*, **157**, 1969, 926,) call attention to the need to know the amount of CH_4 required to reproduce the observed absorption in the 3·1–4·3 μ range. The existing laboratory measurements do not extend to sufficiently large CH_4 abundances. Recently, Margolis and Fox (*Astrophys. J.*, **15**, 1969, 935) and others have resolved and analysed the R-branch of the $3\nu_3$ band of CH_4 at 9050 cm^{-1}, and point out that "an important contribution to the determination of the Jovian methane temperature and abundance would be a measurement of the half-width of the singlet lines in the $3\nu_3$ band, and especially a determination of the line shape".

In the radio region of the spectrum there is still some uncertainty in the location of the CH interstellar line; see, e.g., W. Miller Goss (*Astrophys. J.*, **145**, 1966, 707). Fabry-Pérot interferometer investigations of the $A^2\Delta$–$X^2\pi$ band of CH at 4300 Å results in a interstellar line as consequence of ground-level Λ-doubling at 3030 Mc-s, while van Vleck theory leads to 3400 Mc/s.

In the far IR, the wings of bands of H_2O in its rotation spectrum appear to be too strong. For example, in the 1 mm to 1 cm region one must multiply by four the sum of all absorptions calculated according to the van Vleck formula. It is suggested that this may be caused by the formation of dimers. This is important in the estimation of H_2O abundance in Venus. More laboratory studies are needed of H_2O absorptions over a wider range of temperatures. Also important would be studies of line broadening of H_2O and NH_3 in presence of foreign atoms or molecules, e.g., N_2, CO_2, H_2, He.

The source of 26 diffuse features in the spectrum of interstellar matter is still unknown. The strongest is the well-known feature at 4430 Å. One of a number of suggestions is that they are produced by occluded molecular species on the surfaces of interstellar grains.

J. G. PHILLIPS
Chairman of the Committee

OTHER INFORMATION

Through Mrs Ch. Moore-Sitterly, we have received the following information:

From W. R. S. Garton:

At the Imperial College of Science and Technology, the main advance in the last few years has lain in the development of techniques enabling the extension of absorption spectroscopy of atomic vapors into the range 100–600 Å. The techniques developed have been reported in *Appl. Opt.*, **8** (1969), 919.

Analyses of the p-shell spectra of Na I, K I, Rb I are provisionally complete. The data on Ca I, Sr I and Ba I are being worked up. All the metal vapor spectra previously reported (back in the 1930's) by Beutler have been re-photographed using modern techniques and much greater dispersion. As a result, the spectra of Zn I, Cd I, and Hg I due to excitation of the d-shell and including transitions due to two-electron excitation have been extended. The Tl I spectrum has been greatly extended and the work of Beutler on Rb I and Cs I has been subject to particularly drastic revision. Jointly

with F. S. Tomkins at Argonne, the diamagnetic Zeeman effect has been studied in Ba I (in press in *Astrophysical Journal*) and Sr I; extensive series spectra of Sc I and Y I have been observed in the Schuman UV. In collaboration with Goldberg, Parkinson and Reeves of the Harvard College Observatory, the absorption spectrum of an ion, La II, has been obtained from the middle UV to about 1200 Å. The analysis is in progress.

From R. Wilson:

The Astrophysics Research Unit of the Culham Laboratory, Abingdon, Berkshire (England) continued to be very active in spectroscopy. A report on 'Spectral Classification' prepared by R. Wilson, mainly deals with emission lines from Fe IX to Fe XVIII as well as isoelectronic sequences. Other information may also be found in a report to be published jointly by Science Research Council and the Royal Society, under the title 'Space Research in the United Kingdom 1968/69'.

From C. Newkirk, Jr:

Summaries of the work done at the High Altitude Observatory, Boulder, Colorado, U.S.A., have been published in the Annual Reports of this Institution. The papers of interest for Commission 14 appeared in *Astrophysical Journal*, except a publication by W. J. Wagner and L. L. House on 'A Survey of Current Coronal Visible Line Identifications' (*Solar Phys.*, **5**, 1968, 55–60). These authors have found that of the ~ 100 lines visible at eclipse only about 20 have undisputed identifications. Six new identifications are suggested, based on Wagner's combined laboratory and theoretical study.

At the suggestion of J. Phillips, A. Lagerqvist has reported to us thatat the Institute of Physics of the University of Stockholm more and more work is done in the UV vacuum region. Among other molecules, the spectra of metal hydrides and deuterides are investigated. One research group is studying diatomic spectra of the platinum metals, for example the spectra of PtH, PtD, PdD, PtC, RhC, RuC, IrC, PtO. Efforts are also made on the spectrum of CuO.

Concerning suggestions regarding areas of research activity requiring greater attention than is currently being provided, A. Lagerqvist mentioned (a) UV spectra, (b) Rydberg series, (c) spectra of ionized molecules, (d) intensity and life time measurements of spectral lines, especially in perturbed regions, (e) the mechanism of excitation, (f) hyperfine structure, (g) investigations of very strong perturbations, (h) transition probabilities.

At the Institut d'Astrophysique of the University of Liège (Belgium), B. Rosen and Mrs Denis-Gausset hope to publish in 1970 a new edition of the International Tables of Molecular Constants for diatomic molecules.

The determination of experimental potential functions of np $^1\Pi$ and np $^1\Sigma_\mu^+$ states in H_2, HD and D_2 has been the subject of a publication by A. Monfils (*Bull. Acad. roy. belg., Cl. Sc.*, **54**, 1968, 44).

Measurements on the C_3 4050 group excited in a pulsed low pressure discharge have furnished a first estimation of 300×10^{-9}s for the lifetime of the excited state of this transition (F. Remy, Dr. degree thesis, Univ. of Liège, Oct. 1967).

I. Dubois has studied the spectra of SO_2 (*J. molec. St.*, **3**, 1969, 269), SeO_2 (*Bull. Soc. r. Sci. Liège*, **11–12**, 1968, 562), TeO_2 (*Bull. Soc. r. Sci. Liège*, in press), SiH_2 (*J. Chem. Phys.*, **47**, 1967, 4262, in coll. with G. Herzberg and R. D. Verna, *Can. J. Phys.*, **46**, 1968, 2485).

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