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Chairman of the Committee

COMMITTEE 5: MOLECULAR SPECTRA

Compendia, bibliographies and atlases

The period of time covered by this report saw the appearance of a number of important publications. Of primary importance has been the appearance of the second edition of *Spectroscopic Data relative to Diatomic Molecules (1)* prepared by an international team of spectroscopists under the direction of B. Rosen. About 700 diatomic molecules are covered. For each molecule most of the following are included: mode of production, wavelengths and classification of vibrational band heads, molecular constants, dissociation energies, perturbations, predissociations, ionization potentials, transition probabilities, and a detailed bibliography to 1969. As a follow-up to this enormous task, a group is preparing to produce annual critical abstracts and up-dates. A program is being written at Stockholm to catalogue data from this table, both by molecule and by wavelength. Several bibliographies have appeared or are in preparation. Carlos Suarez at La Plata has compiled via computer a *Bibliography of Spectra of Diatomic Molecules, 1960–1970*. It is in four parts; a few polyatomic molecules are also listed. The International Union of Pure Applied Chemistry publishes a *Bibliography on the High Temperature Chemistry and Physics (2)* which includes many interesting references to laboratory techniques, specific heats, transition probabilities, etc. T. M. Dunn at Michigan and T. Larsson and H. Neuhaus at Stockholm are maintaining bibliographies of hyperfine structures in diatomic molecules, David R. Lide of the Office of Standard Reference Data, N.B.S., has called attention to the new *Journal of Physical and Chemical Reference Data*, which will include compilations and reviews of interest to molecular spectroscopists. The bi-monthly Berkeley News letters are continuing; the mailing list has grown to cover 400 spectroscopists in various countries. Each bi-monthly issue includes a bibliography of papers on diatomic and simpler polyatomic molecules appearing in over 30 journals. R. W. Nicholls has continued the publication of the series of Identification Atlases of Molecular Spectra, the most recent covering the CO Fourth Positive System, VO, and the CN Red System; an atlas on the CN violet system is in preparation. Publication of the CRESS reports by Nicholls and his collaborators has continued; they include data on Franck-Condon factors and related quantities for a long series of band systems. Lifetimes in gaseous diatomic molecules have been discussed in a recent article by Anderson (3). Finally a number of monographs of great value have appeared. They include: *Rotational Structure in the Spectra of Diatomic Molecules* by I. Kovacs (4), *Far-infrared Spectroscopy* by Moller and Rothschild (5), *Microwave Molecular Spectra* by Gordy and Cook (6), *Rydberg series in Atoms and Molecules* by Duncan (7), *An Introduction to Molecular Spectroscopy* by Herzberg (8), *Low Temperature Spectroscopy* by B. Meyer (9) and *Revised Tables of Diatomic Molecular Constants* by K. P. Huber (10).

Molecular data

Even if the discussion is limited to molecules of astrophysical interest, the research that has been completed is much too extensive for full coverage here. Reference should be made to the bibliographies listed above. A selection of recent analyses includes the following.

(a) *Electronic band analyses and constants for diatomic molecules*

On molecules involving carbon, Fay *et al.* have improved the molecular constants of the Red System of CN (11), while Kepa and Rytel have found a new band system ($\pi-\pi$) of CO (12). An absorption spectrum of CO in the 600–1020 Å region has been investigated by Ogawa and Ogawa (13), and isotopic CO bands by Simmons and Tilford (14) and Kepa *et al.* (15). Green (16) has calculated potential energy curves for CH⁺, while Meinel (17) reports a possible new C₂⁺ spectrum. Among the diatomic oxides, Miescher has continued his extensive investigations of the absorption spectrum of NO (18) while Brown *et al.* have studied infrared magnetic dipole transitions of NO (19). Molecular constants of OH and O₂ have been calculated by Mizushima (20) and Welch and Mizushima (21). Moore and Richards (22) have re-analysed the $A^2\Sigma^+-X^2\pi$ system of OH. The vacuum ultraviolet spectrum of SiO has been investigated by Elander and Lagerqvist (23), while Cornet and Dubois report on a new electronic transition in SiO (24). Green has analysed the rotational structure of the $C^2\pi-X^2\pi$ transition of LaO (25), and investigated low-lying electronic states of LaO, YO, and ScO (26). A new $^1\Sigma-^1\Sigma$ band system of TiO has been reported by Phillips and Davis (27) and extended by Lindgren (28), and a further ($^1\Delta-^1\Delta$) TiO system has been reported by Linton (29). Satellite bands of the γ -system of TiO have been analysed by Phillips (30). The ionization potential of H₂ has been re-examined by Herzberg and Ch. Jungen (31); Stephens and Dalgarno have calculated the spontaneous radiative dissociation in H₂ (32), while Crosswhite (33) has edited the hydrogen molecule tables of G. H. Dieke.

(b) *Transition probabilities, lifetimes, intensities*

Aert Schadee has investigated the normalization of the Hönl-London factors and the definition of the molecular electronic transition moment (34). A great amount of work has been done recently on CO and CO⁺. In the case of CO, Ajello has measured emission cross-sections by electron impact in the 1260–5000 Å region (35); the intensity of the Cameron system by Pilling, Bass and Braun (37) and the infrared rotation-vibration spectrum by Roux *et al.* (38) and Lowder (39). Oscillator strengths in the CO⁺ comet tail system have been derived by Jain (40) and its electronic transition moment by Maier and Holland (41). Judge and Lee (42) have recently carried out an extensive computation of electronic transition moments and absolute cross sections for a number of CO⁺ transitions. Collisional transition probabilities and Franck-Condon factors for excited states and transitions of CN have been calculated for the red system of CN have been carried out by Johnson, Marenin and Price (45) and Querci *et al.* (46); the latter also include other systems of CN and C₂. Among the large number of recent studies of various aspects of the spectrum of H₂, there has appeared a calculation of infrared emissivities of H₂ and HD carried out by Dalgarno and Wright (47). The intensities and transition probabilities of electronic systems of NO have been investigated by Copeland (48), Michels (49), Hasson and Nicholls (50), and Farmer, Hasson and Nicholls (51), while work on its infrared rotation-vibration spectrum has been carried out by Bubert (52) and Moskalenko and Mirumyants (53). Also in the infrared, the intensities of OH bands have been observed by d'Incan, Effantin and Roux (54) and Murphy (55). Hasson and Nicholls (56) and Jarman (57) have observed O₂ ultraviolet bands and calculated Franck-Condon factors for the Herzberg system. Among the metallic oxides, mention should be made of an investigation of absorption coefficients in the infrared vibration-rotation spectrum of FeO by Fissan and Sulzmann (58), a singlet electronic system of SiO by Smith and Liszt (59), AlO by Michels (60) and Johnson, Capella and Broida (61), and LaO by Murthy and Murthy (62).

(c) *Polyatomic molecules*

The rapid extension of astronomical researches into the infrared and radio regions has focussed increasing attention of polyatomic molecules, either known to exist in the atmospheres of late-type stars or in interstellar matter, or suspected of being of potential importance. The following is only a sample of the numerous investigations that have been carried out recently.

The high resolution infrared spectra of isotopic species of CO₂ have been investigated by Oberly

(63, 64); improved constants for this molecule have been calculated by Val (65), and its $2.7 \mu\text{m}$ band has been treated by Kunitomo and Ninai (66). Measures of relative intensities in electronic bands of CO_2^+ have been carried out by McCallum and Nicholls (67). The bending frequency of the C_3 molecule has been measured by Liskow *et al.* (68), while the infrared spectrum of O_3 has been the subject of a number of investigations by Lichtenstein *et al.* (69), Brewer and Wang (70) and Barbe, Secroun and Jouve (71). For NO_2 there are compilations of molecular constants by Blank (72) and Ramaswamy and Shanmugan (73), and oscillator strengths by Gangi and Burnelle (74). The infrared spectrum of N_2O has been investigated by Smith *et al.* (75), Tien, Modest and McCreight (76). Lowder (77), Margolis (78), Sokoloff and Javan (79). Bands of HCN at 14 microns have been described by Yin and Rao (80) while the microwave spectrum of HCO has been investigated by Bowater, Brown and Carrington (81). Isotopic bands of H_2O in the infrared have been reported by Williamson, Rao and Jones (82) and Steenbeckelers and Bellet (83) and the submillimetre spectrum of H_2O by de Lucia *et al.* (84). The spectrum and structure of the HO_2 free radical have been described by Jacox and Milligan (85).

RESEARCH IN PROGRESS

(a) *From the National Research Council of Canada*

(reported by G. Herzberg and A. E. Douglas)

The ultraviolet emission and absorption spectrum of HF has been studied by di Lonardo and Douglas and much more complete information has been obtained than available up to now. Similarly the absorption spectrum of F_2 in the vacuum ultraviolet has been studied by Douglas and Raymond. The ground state constants of F_2 have been much improved.

In our program of studies of molecular ions H. Lew has succeeded in observing an extensive spectrum of H_2O^+ which in many ways is similar to the spectrum of NH_2 . Provisional values for the ground state constants have been obtained. They fit well with the constants for the Rydberg states of H_2O which J. W. C. Johns is continuing to study. H_2O^+ is an ion that almost certainly will be discovered sooner or later in the interstellar medium and possibly in comets.

The Lyman and Werner bands of D_2 in the vacuum ultraviolet have been studied in absorption and emission, and much improved values for the molecular constants in the ground state and the excited states have been obtained by Bredhol and Herzberg. Also a study of the vibrational levels near the dissociation limit of HD has been initiated by Dabrowski and Herzberg.

(b) *From the National Bureau of Standards*

(reported by Karl G. Kessler and Don Johnson)

Spectroscopic work at NBS is going on in the optical region. Theoretical studies on molecular topics are also being carried out to compliment the experimental work.

In the optical region, considerable effort is still being spent on electronic spectra of diatomic molecules. An extended systematic analysis by J. D. Simmons of the CO absorption bands to the low lying valence states has recently been concluded. The seven excited valence states involved have been identified as belonging to two electronic configurations: $\pi^3\pi^*$ and $\sigma\pi^*$. A re-examination of the vacuum ultraviolet emission spectrum of CO has led to some interesting results. Two emission systems identified with CO for many years have now been assigned to N_2 . Two new band systems for CO have been located and the accidental predissociation in the $E^1\pi$ state of CO has been confirmed.

P. H. Krupenie has completed an extensive critical review of the electronic spectrum of O_2 . A similar critical review of molecular nitrogen is in progress by Krupenie in collaboration with A. Loftus of the University of Oslo.

Several polyatomic molecules of particular interest for interstellar work have been studied in the microwave region. D. R. Johnson and F. J. Lovas have recently assigned the rotational spectrum

of CH_2NH . Detailed centrifugal distortion analyses of the microwave spectra of H_2CS and NH_2CHO have been carried out by Kirchhoff and Johnson.

Critical reviews of laboratory microwave spectra of several interstellar molecules have been undertaken with an aim at reliably predicting all rotational transitions in those molecules which might be expected to be detectable with radio telescopes. Kirchhoff, Lovas and Johnson have completed such reviews for H_2CO , H_2CS , NH_2CHO , and CH_2NH . A collaborative effort with R. Lees of the University of New Brunswick has produced a similar review of CH_3OH . HCN and OCS are presently under review by A. G. Maki. Krupenie and Lovas are nearing completion of similar reviews of CO, CS and SiO.

Several molecules of astronomical interest are being studied under high resolution in the infrared. W. B. Olson has recently determined ground state rotational constants for CH_3D and is presently analysing the γ_2 band of CH_3D at 2200 cm^{-1} . Ground state rotational constants have also been determined for SiH_3D by R. W. Lovejoy and W. B. Olson. NO_2 is currently under investigation at high resolution by W. J. Lafferty and R. L. Sams. Maki and Sams are using a high temperature oven in order to observe HCN transition in highly excited rotational and vibrational levels. Work less directly applicable to astronomy is underway on AsH_3 , PH_3 and CS_2 .

(c) *From the University of California, Berkeley*

(reported by J. G. Phillips and S. P. Davis)

Measures and analyses of the high dispersion rotational structures of TiO from 4000 \AA to $1.1\text{ }\mu\text{m}$ are completed. Over 35000 identifications have been made in 7 band systems. The identifications are available on cards, IBM computer print-outs, and eventually on tapes and microfilm. These analyses have been used to derive improved TiO molecular constants. A similar program is being initiated on ZrO. Preliminary tests give assurance that we can readily resolve the more crowded rotational structure and apply the same programs of reduction and analysis that have proved so successful for TiO.

A program of measurement of lifetimes of selected levels in four systems of TiO has been initiated using an electric furnace and a fluorescence technique. Relative transition probabilities of bands of ZrO in the $4000\text{--}7000\text{ \AA}$ range are being measured on furnace photoelectric scans and photographs.

(d) *From the Astronomical Institute at Utrecht*

(reported by Aert Schadee)

Schadee has been working on the normalisation of Hönl-London factors and the definition of the molecular electronic transition moment. Furthermore prompted by high dispersion sunspot spectra, he is trying to find out from the literature, what kind of Zeeman splittings are to be expected for dominant molecules.

(e) *From the Eidg. Technische Hochschule Zurich*

(reported by K. Dressler)

We have begun work on a deperturbation study of the intensity distribution in the absorption spectrum of NO. The final aim of this work is the computation of synthetic absorption spectra of NO at different temperatures and resolutions. This is of interest, e.g. for studies of the upper atmosphere. Indeed, we are already in contact with Dr Wofsy at the Smithsonian Astrophysical Observatory in Cambridge, Mass., who needs such data in calculations of photo-dissociation rates and UV reflection in the upper atmosphere.

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