been given for neutrals (158) and ions (Burgess, unpublished); and results have been tabulated for  $n \rightarrow n + 1$  transitions in H (156). The method is least reliable when  $\Delta E$  is large and when f is small.

Another approach is based on classical theory (Gryzinski, (62); Burgess, (64)). This is best when  $\Delta E$  is not small. The method of Burgess and of Ochkur (133a) may be used for intercombination transitions.

# 111. Experimental Work

The main technical advance has been in obtaining improved energy resolution. Many cross section-energy curves show fine structure. References to experimental work on H, He, alkalis and other atoms are given in (64).

#### IV. Ionization

Taking account of all experimental results, Heddle and Seaton (64) give what they believe to be the best estimate of the H ionization cross section. Recent experimental determinations have been made for O (52). N (162) and alkali atoms (19). A major achievement has been the measurement of cross sections for positive ion ionization, He<sup>+</sup>, Ne<sup>+</sup> and N<sup>+</sup> (41).

Improved techniques of calculation have been developed (58, 142), and accurate calculations have been made for hydrogenic ions (155) and for  $O^{4+}$  and  $O^{5+}$  (169).

## v. Recombination

Burgess (21) shows that dielectric recombination has a large rate coefficient at high temperatures.

### A SYNOPSIS OF MOLECULAR INTENSITIES

## (Committee 2, continued)\*

## R. W. Nicholls

#### 1. Introduction

Although this review is concerned mainly with intensity problems, it will not be out of place to mention some important identification aids which have recently become available:

The third edition of '*The Identifications of Molecular Spectra*' by Pearse and Gaydon (139) has been published, as has '*A Spectrophotometric Atlas of CH from* 3000-5000Å' (6). The Bumblebee Report on OH has now appeared in the open literature (38) as have two very useful compilations of band head wavelengths by Wallace (173). An identificational Atlas of Molecular Spectra is in preparation (129).

Three general review papers on the concepts of molecular intensities may be mentioned (125, 133, 164a).

# II. Intensity Measurements of Molecular Spectra

Relative or absolute intensity measurements in emission or absorption from photographic or photo-electric recording techniques have been reported for the following cases:

O<sub>2</sub> Schumann Runge (63, 97): O<sub>2</sub> Herzberg Continuum (40), NO (33, 179).

OH Vibration-Rotation (27, 57): OH Violet Bands (99).

 $N_2$  Vegard-Kaplan (26):  $N_2$  Second Positive,  $N_2^+$  First Negative (174).

SiN (166): CN Violet (50): CO (109): C<sub>3</sub> (18).

\*Reference numbers in parentheses refer to the general bibliography which follows the report of the Commission.

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In many of these cases the data have been used to study the variation of the electronic transition moment with internuclear separation for the transition, and thereby to infer band strengths and other related transition probability parameters.

The interpretations imply that each molecule acts as if isolated from its environment. Some recent studies on measurements of the intensity ratios of pairs of  $N_2$  bands which arise from the same upper level, show that the ratio is not entirely independent of current density and, therefore, of excitation environment (170, 143). Although the effect is small it indicates that the isolated molecule concept should be treated with care.

#### **111.** Molecular Lifetime Measurements

The direct measurement of molecular lifetimes by the delayed coincidence technique, applied to CO<sup>+</sup>, CH and NH, and N<sub>2</sub>O<sup>+</sup> has been extended to CN (13).

The lifetime of the metastable  $A^{3}\Sigma$  state of N<sub>2</sub> has been inferred from accurate concurrent measurement of intensities in absorption of the First Positive system and in emission of the Vegard-Kaplan system (25).

### IV. Re-interpretation of Past Intensity Measurements

Molecular lifetimes or absolute intensities in absorption have been used in a number of cases to place relative emission intensities on an absolute basis. The following molecules have been treated:

$$N_2$$
 and  $N_2^+$  (127): CO+ (124): CN, OH (130).

An intercomparison has been made of all the known intensity measurements (relative and absolute, emission and absorption) of the beta and gamma systems of NO (106). It has been possible to derive an electronic transition moment function which fits both systems and to produce extensive arrays of absolute transition probability parameters for the transitions. A similar study has been made for  $O_2$  (Schumann-Runge) (107).

## v. Vibration-Rotation Interaction

The effect of vibration-rotation interaction upon molecular intensities has been studied theoretically (54, 83) and experimentally for the CO vibration-rotation spectrum (12, 95).

## v1. Studies of Band Profiles

The increasing use of hot optically-thick light sources has given rise to a number of papers which deal with the effects of band and line profiles upon total band intensity (108, 137, 164). The question of unoverlapped fractions of extensive bands has also been considered (153).

### VII. Absorption and Emission from Hot Molecular Gases

Spectral absorption and emission from hot gases has been of increasing interest during the past three years. Experimental measurements have been made of  $N_2$  (1), air (24), and  $CO_2$  (164b); NO (164b) has been discussed theoretically and the overall problem reviewed (3, 141).

### VIII. Franck-Condon Factors and other Derived Quantities of Vibrational Wave-Functions

The correct interpretation of intensity measurements on molecular spectra requires that a number of theoretical parameters derived from vibrational wave-functions be available. The most important of these parameters is the Franck-Condon factor. Numerous arrays of these (both limited in extent in some cases and extensive in others) have been published. The old analytic approximations to the Franck-Condon factor are outdated and have been replaced in large degree by direct computer evaluation. A number of molecular potentials have been tried, the most common being the Morse potential and the 'realistic' Klein-Dunham potential (see next section).

On the basis of a Morse potential, extensive computer-evaluated arrays have been obtained to high quantum numbers for band systems of:

 $N_2$  and  $N_2^+$  (122, 123). AlO, MgO, SrO, BaO, VO, NO (126): CO<sup>+</sup> (124): Many vacuum ultra-violet radiative and excitation transitions (125):  $I_2$  (128): CN (131):  $C_2$ .

Limited arrays based on analytic approximations have been computed for SiO (110): CO (160): AlO (167): RbH (81): VO (135).

Precise computer evaluation of vibrational wave-functions for Klein-Dunham potentials (86) has been carried out for a number of cases (87).

The geometry in the v', v'' plane of Condon loci has also been studied (132).

## **IX.** Molecular Potentials

A number of workers have continued the tabulation of Klein-Dunham realistic molecular potentials for selected diatomic molecules: (84, 85, 161, 168). Numerical studies of vibrational potentials appropriate to these wave-functions have also been made (82, 86).

## GENERAL WORK ON MOLECULAR SPECTRA

In addition to the above report by Nicholls, general investigations on molecular spectra have been carried on. In Berkeley, Phillips and Davis have continued the large program on diatomic molecules of astrophysical interest. Conversion to an IBM 7090 computer has been completed. The bi-monthly Newsletter continues to serve as a progress report for spectroscopists who wish to be on the mailing list.

The CN lines account for at least 95 per cent of the absorption lines in this region of the spectra of carbon stars. The Monograph on red CN has been published (35).

Programs have been written for the electronic computer, which calculate rotational line intensities and absorption line profiles in the highly blended CN molecular spectrum of the carbon stars. This program will make it possible to study the effect of the blanketing of the atmosphere of a star by CN, and also to determine the  $C^{12}/C^{13}$  isotope ratio in the atmospheres of various carbon stars.

Investigation of C<sub>2</sub> is in progress. Between 4200 and 6700 Å more than 30 bands have been detected, some with branches extending to N = 80.

TiO has been observed from 4462 to 8000 Å in an electric furnace operated between 2373° K and 2573° K.

AlO is being investigated in collaboration with M. A. Poggio of the University of La Plata in Argentina.

A detailed analysis of 30 bands of HgH will comprise the second Berkeley Monograph.

An unexplained large scatter in the published wavelength lists of Th at wavelengths smaller than 5000Å, used as a comparison spectrum, should be checked.

Herzberg reports work on vacuum ultra-violet molecular spectra, that are of continuing interest to the astrophysicist. Detailed investigations of the Lyman bands of  $H_2$  were completed in 1959. Since then similar investigations of the Lyman bands of  $D_2$  have been made but they have not yet been completed. In addition, the absorption of  $H_2$  as well as of HD and  $D_2$  at still shorter wavelengths down to the absorption limit of 849Å, has been studied.

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Another important spectrum to be expected in the far ultra-violet is that of  $H_2O$ . This has been studied under very high resolution by Johns. Similar spectra of  $H_2S$  have been obtained by Johns but not yet published. Another spectrum that might be of importance is that of  $NH_3$ which starts to absorb below 2200Å giving rise to a large number of discrete bands. This spectrum was studied at high resolution by Hollas and Douglas, and Douglas.

Recently the vacuum ultra-violet absorption of CH has been studied. This molecule has fairly strong absorption bands at 1690, 1550, 1370 and 1271Å. Of these the absorption at 1370Å is the strongest and is likely to occur in many astrophysical sources. Quite recently a few absorption bands of  $C_2$  between 1400 and 1300Å have been found, but these spectra have not yet been analysed. Finally, one might mention the strong absorption spectra of CH<sub>2</sub> and CH<sub>3</sub> which occur below 1500Å. There is also a weaker absorption of CH<sub>3</sub> at 2160Å which might conceivably be of astrophysical importance.

A number of other molecular spectra in the vacuum ultra-violet have been investigated, but they are not likely to be of astrophysical interest.

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NH <sub>3</sub>	Douglas, A. E., Hollas, J. M. Can. J. Phys., 39, 479, 1961.
NH <sub>3</sub>	Douglas, A. E. Disc. Far. Soc. Lond., no. 35, 158, 1963.
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CH	Herzberg, G., Johns, J. W. C. (to be published).

Mme R. Herman and her collaborators at Meudon report investigations on selected molecular spectra as follows:

0 <sub>2</sub>	Schumann-Runge bands extended to 5700 Å (68).
$O_{2}^{+}$	New bands of the first negative system observed and analyzed; second negative
-	system being studied (66, 96, 176).
$N_2$	Preliminary results obtained on intensities of first and second positive systems
	as a function of the mean energy of the electrons (61).
$N_{2}^{+}$	First negative system observed in emission in phosphorescence (65, 66).
OH, OD	Studies of suitable experimental conditions for observing high level systems;
	transition probabilities calculated (48, 49).

A program on unstable molecules is also in progress.

In Liège, research activity, according to Monfils, includes a detailed study of molecular hydrogen absorption spectra. Refined values of the constants will soon be published for HD,  $D_2$ , and  $H_2$  (115, 116).

## GENERAL WORK ON ATOMIC SPECTRA

At Meudon some experimental work on atomic spectra is also reported by Mme R. Herman.

(a) Infra-red observations: Between  $1.6\mu$  and  $3.7\mu$ , 24 new lines of Cs1 have been observed and classified; 13 of Cd1 and 2 of HeI (159).

(b) Stark Effect: The observed dissymetry of  $\lambda$ 7601 of Kr1 may be attributed to Stark Effect (67). Stark constants for H have been calculated automatically by an iteration method (42).