WORKING GROUP 5: MOLECULAR SPECTRA

A. *Compendia, Bibliographies and Atlases*

Molecular spectroscopic activity, and its literature, has continued to proliferate strongly during the reporting period. There has been much work over the entire wavelength range: microwave - extreme ultraviolet. The impact of the methods of laser spectroscopy on the field, and developments in molecular lasers have continued to provide a great stimulus to molecular spectroscopic research. There has also been increasing recognition of the need for fundamental spectroscopic data of all kinds in astrophysical, atmospheric and enviromental research applications. The scope of contemporary interests is displayed in the programme books for the symposia on Molecular Spectroscopy held annually at the Ohio State University. For the past three years the literature of the molecular spectroscopy has been so prolific that it is impossible to make a definitive review even of the astrophysically important contributions beyond brief citations. Important trends are indicated below. Literature citations have been principally compiled from the reports received from individual workers in Centres of Research on molecular spectra.

The bi-monthly Berkeley Newsletter (1) compiled by Phillips and Davis from more than 30 journals continues to be distributed to about 500 workers. It gives most valuable access to the literature of the spectra of small molecules. Recent copies reference 200-300 papers, books, etc. The wide need for reliable compilations, for a critical assessment of molecular data has been increasingly emphasized during the past few years. Herzberg and Huber (2) report the publication of a long anticipated volume "Constants of Diatomic Molecules" which makes a critical assessment of the literature and significantly updates the tables of Herzberg's "Spectra of Diatomic Molecules", published in 1950. Hsu and Smith (3) have made an important review of spectral data of visible and ultraviolet diatomic molecular spectra of astrophysical interest. Nicholls (4) has reviewed transition probability data for astrophysical molecules. Lofthus and Krupenie (5) have compiled data on the spectrum of N_2. The identification of molecular spectra has continued to remain an important problem. Pearse and Gaydon (6) have published in 1976 the fourth edition of "The Identification of Molecular Spectra". Kopp, Jansson and Rydh (7) have published a table of band features of diatomic molecules which is a supplement to the 1974 edition, cf. the 1975 report of this Committee. Spectral atlases continue to be produced. Hsu, Monts and Zare (8) have published a spectral atlas of NO_2. Park (9) has produced a spectral atlas of infrared absorption lines and Nordstrom, Shaw, Skinner, Calvert, Chan and Uselman (10) have published an atlas of air absorption in the infrared between 700 and 2300 cm^{-1}. Roney et al (11) and Benedict (12) have recently commented on the data in the Air Force Geophysical Laboratory atmospheric absorption line parameter compilation. Two important books on Molecular Spectroscopy have recently appeared: "Diatomic Molecules, Results of ab initio Calculations" by Mulliken and Ermler (13) and "Molecular Symmetry and Spectroscopy" by Bunker (14).

B. *Molecular Data*

During the past three years there has been a continued emphasis on diatomic molecules of astrophysical, atmospheric and laser importance. Herzberg and Huber's "Constants of Diatomic Molecules (2) is an invaluable contribution to this area. Whiting et al. (15) have made recommendations for clear definitions of transition moments and intensity factors in the spectra of diatomic molecules. The diagnostic applications of molecular spectroscopy to stellar atmospheres calls for a continuing critical assessment of the thermochemical data available for stellar molecules. The need for better data in this field has been strongly emphasized by Sauval and Tatum. Similarly high quality data on excitation cross-section data for diatomic molecules are needed. Ames and Huebner (16) report studies on emission cross-sections for rotational transitions. There has been continued interest on potential energy curves for diatomic molecules. Kuriyan and Pritchard have made numerical studies

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on potentials H_2(17,18). Schadee reports studies on the Zeeman effect in electronic transitions of diatomic molecules (19). Hefferlin (20) has continued studies on a periodic table for diatomic molecules. There has been a continuing research effort on *ab initio* quantal calculations on the properties of many diatomic molecules. Important developments in this field are being made at the NASA Ames Research Center, at the Argonne National Laboratory and the IBM Research Center San Jose.

I. Electronic Band Analyses and Constants of Diatomic Molecules

Coxon and Sastri are making a comprehensive attempt consistently to fit all of the available scientific data on OH by one model. Tatum continues analyses on bands of TcO. Dressler reports analyses of H_2 (21), N_2 (22) and N_2^+ (23) states. Barrow reports studies of CuF (24), FeF (25), CeO, SiS and FeO. Kotlar has made an extensive analyses of the CN Red Band System using Berkeley data (26). Linton reports analyses of TiO systems (27,28), SiO systems (29,30) and on one system of YO (31). Jordan (32) reports collaborative studies of CO fluorescence and lines of H_2 in the extreme UV solar spectrum (33). Lew (34) has made analyses of singlet systems and measurement of dissociation energy of NH and ND. Brown reports studies on the He_2 (35) and Ag_2 (36) molecules. Benesch reports high resolution studies on N_2^+ bands (37) and infrared N_2 bands (38,39,40). Lindgren reports analyses of MgH and MgD spectra (41) and identification of FeH in the spectra of M dwarfs and S stars (42). Ramsay reports analyses of the vibration-rotation spectrum of HD (43) and a r-analysis of the ClO system (44). Shaw (45,46) reports methods of band analyses using computer graphics display terminals. Leach reports analyses of CS bands (47).

II. Transition Probabilities, Lifetimes, Intensities

Two sets of suggestions for uniformity of definitions concerning transition probability data for diatomic molecules have been made recently. Schadee (48) has proposed uniform definitions of band strengths of diatomic molecules and Whiting et al. (15) have proposed uniform definitions for Hönl-London factors and electronic transition moments for diatomic molecules. Numerous high quality measurements of lifetimes have been made for the upper states of many transitions of astrophysical interest. These include extensive work by Erman and colleagues in Stockholm using the high frequency deflection technique (49) which allows lifetime measurements of individual rotational levels. Erman reports work on CH^+ (50), other hydride ions (51), other hydrides (52,53,54), I_2 (55), C_2 (56), N_2^+ (57) and NO (58). Instrumental and review aspects have been discussed (59,60,61). Predissociation and perturbations studies have been made (62,63,64,65). Thrush et al have made lifetime measurements on excited BO and BO_2 (66). Llewellyn (67) reports lifetimes measurements on OH and excitation kinetic of the IR atmospheric O_2 bands (68) and quenching of OH (69). Leach et al (70) report lifetime measurements on C_2. Linton (71) reports lifetime measurements on TiO. Davis also reports lifetime measurements on the TiO α and β systems (72,73). Sulzman has made shock tube measurements of oscillator strengths of TiO α and γ bands (74), and of vibration-rotation bands of AlO (75). He reports high temperature absorption coefficient measurements on methane (76) and non-LTE spectral absorption coefficients for vibration-rotation bands of diatomic molecules (77) and on other electronic bands of diatomic molecules (78). Benesch reports absolute oscillator strength measurements on bands of N_2 (79). There have also been a number of photoelectron spectroscopy measurements of cross-sections for various astrophysical band systems. Marr (80,81) reports such measurements for N_2 using synchrotron radiation, Samson et al have made photoelectron studies of H_2 (82), N_2 (83), O_2 (84), O_2^+, N_2^+, CO^+(85), CO_2 (86), CO (87), O_2^+ (88). Gattinger reports synthetic spectral studies of O_2^+ (89), O_2 (90) and N_2(91) in the spectrum of the aurora. Shaw reports intensities and widths of H_2O (92) and N_2O, CO_2, CO and H_2O (93). Carver (94) reports oscillator strengths and line-widths for O_2 Schumann-Runge bands. Arnold et al (95) have made shock tube measurements of SiO transition moments. Smith et al. report refractive index measurements on H_2, He, O_2, CO and Kr

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(96). Johnson reports transition probability studies of N_2 (97). Stoicheff reports laser excited fluorescence studies on CO and lifetime measurements of perturbed levels (98). Ab initio theoretical studies on SiO (99), C_2 Swan Bands (100) and HOCl (101) are reported by Arnold. Rumble (102) has made studies on bounds on the oscillator strength of H_2. Dalgarno reports calculations of oscillator strengths (103) for Li_2 and Na_2^+(104) for alkali hydrides (105), of potential curves for Li_2 (106), for potential curves for two electron systems (107), and vibration-rotation transition probabilities for H_2 (108).

III. Polyatomic Molecules

A wide variety of polyatomic studies in the radio frequency, infrared, visible, and ultraviolet regions of the spectrum have been reported. Ramsay reports observations on NH_2 (109), glyoxal (110), diacetylene (111), formaldehyde (112), and NH_2 (113). Oka describes detection of cyanohexatriyne (114), and observations on cyanodiacetylene (115,116). He reports work on forbidden infrared transitions using two photon laser resonance spectroscopy (117). Observations were made on NH_3 (118, 119,120) and HCO (121). Lees reports microwave double resonance studies on OCS (122,123, 124), on methanol (125,126), on methane (127), and on silane (128). Gerry reports microwave studies on isocyanic acid (129), silane (130), cyanacetylene (131), cyanogen isocyanate (132), propyolic acid (133), and HNCS (134). Lutz reports on high resolution infrared studies on methane with application to atmospheres of planets (135,136,137,138). Leach reports studies on the optical spectra of molecular ions (139), CO_2^+ (140), and CS_2^+ (141). McDowell reports continued work on the photoelectron spectroscopy of small molecules (142,143) such as the diazenes and the imines which are of potential astrophysical interest, although they have not yet been identified as interstellar molecules due in part to lack of knowledge of their microwave spectra.

RESEARCH IN PROGRESS

A. *From the National Research Council of Canada*
(reported by G. Herzberg and A.E. Douglas)

Spectroscopic studies of molecules of astronomical interest continue to be the major interest of the laboratory.

Absorption and emission spectra of HD in the vacuum uv have been investigated (156), the emission spectrum of H_2 is being remeasured with greater accuracy. Experimental studies of the infrared vibrational spectrum of HD (161) and the rotational quadrupole spectrum of H_2 (182) have been completed together with theoretical studies of the HD spectrum (158) (180). The vacuum ultraviolet absorption and emission spectra of the diatomic molecules F_2 (159) and Cl_2 (151) have been investigated and the near ultraviolet spectrum of ClO has been re-investigated in more detail (157). The absorption spectrum of BeH has been described (154) and some of the perturbations in the $B^2\Sigma$ state of CN have been explained (150). Two review papers on the spectrum of NO have been published (164) (166). A number of papers have been published on the electronic spectra of the diatomic molecular ions HF^+ (145), NO^+ (146), O_2^+ and N_2^+ (169) and on the calculated infrared spectrum of HeH^+ (170). A detailed analysis of the electronic spectrum of H_2O^+ (163) and a measurement of the lifetime of the excited state (149) have been published. An extensive study of the electronic spectrum of $HeNe^+$ has just been completed (184). Further investigations of the electronic spectra of the polyatomic molecules NCO (144), NH_2 (147) (148) (162), NO_2 (174), HNO (165) and C_4H_2 (171) have been reported. Considerable effort has been devoted to the study of the infrared spectra of molecules by the laser-Stark and laser-Zeeman methods since this work can give accurate frequencies of infrared lines which are of interest for infrared astronomy. Studies have been reported on the spectra of H_2CO (173) (178), HDCO (168) (183), NO (153), HCO (177) (179), HNO (167), HO_2 (181) and work is in progress on H_2CNH. In addition double resonance and two-photon experiments have given similar information on the infrared spectra of NH_3 (160) (175), NO (176) and SiH_4 (152) (155). A study

of the absorption spectrum of CH_3D in the 6000-12000 Å range has been published (172).

B. *From the National Bureau of Standards*
(Reported by Frank J. Lovas)

a. Data Assessment, Reviews, Atlases

The molecular spectra data center at NBS has a continuing program to develop critical reviews, some of which specifically deal with the spectra of interstellar molecules. Some of these are carried out at NBS and others by spectroscopists at other institutions. Recent critical reviews published in the J. Phys. Chem. Ref. Data series "Microwave Spectra of Molecules of Astrophysical Interest" cover the microwave spectra of CH_3CHO (185), HNCO (186), SiS (187), OH (188), HCCCN (189), and CH_2=CHCN (190). The major feature of these reviews is to provide the fundamental data needed for identifying and interpreting interstellar observations. Predicted spectral lines are given in addition to the observed frequencies in order to provide complete frequency coverage. Work is in progress on CH_3CCH, and CH_3CN (191), HCOOH (192), $HCOOCH_3$ (193), CH_3OCH_3 (194). A new compilation entitled "Recommended rest frequencies for observed interstellar molecular lines", is close to completion (195). An extensive critical review of the microwave spectra of 54 triatomic molecules has been completed and will appear as Part II of the "Microwave Spectral Tables" (196). The review contains spectral data on the interstellar molecules H_2O, H_2S, OCS, HCN, HNC, HNO, HCO, HCO^+, HN_2^+ and SO_2. A new NBS compilation on high resolution infrared has been started by W. Lafferty and A. Maki. The first review will treat selected diatomics: CO, CS, ClO and the hydrogen halides. An extensive compilation of the NO spectrum is also in progress by Guelachvili. In the area of electronic spectra an atlas of the absorption spectrum of NO (197), and a definitive review of the spectrum of N_2 (198), have been published recently.

b. Molecular Data

1) Microwave region

Isotopic forms and the molecular structure of CH_2NH has been studied (199). Measurements of the millimeter spectrum of C_2H_5CN assisted its identification in interstellar sources (200). The laboratory microwave spectrum of NH_2CN has been reported (201). New measurements of the microwave spectrum of $^{14}N^{32}S$ and $^{14}N^{34}S$ have been completed (202).

2) Far infrared region

Laser magnetic measurements of the rotational spectrum of CH have been carried out at NBS-Boulder (203). Work is now in progress on CH_2 by K. Evenson and coworkers.

3) Infrared region

The 2-0 vibration-rotation bands of $^{12}C^{32}S$ and $^{12}C^{34}S$ near 2530 cm^{-1} have been reported (204) and a high resolution study of the 1-0 bands with a diode laser spectrometer has just been completed (205). A high resolution study of HNC in equilibrium with HCN has been completed by Maki and Sams (206). Jacox has published a matrix isolation study of the infrared spectrum and structure of the CH_3 free radial (207).

C. *From the University of California, Berkeley*
(Reported by J.G. Phillips and S.P. Davis)

1. Molecular Analyses

High resolution Fourier transform spectroscopy has been used to study the emission spectrum of TiO between 4000 A and 3 μm. The analysis of the ψ-system has

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been completed. About 3000 lines from 25 bands have been identified. Molecular constants have been calculated. Band intensities agree well with predicted Franck-Condon factors and known isotope abundances. 19 new bands of the ($^1\Pi$-$^1\Sigma$) system of ZrO have been identified from 5849 A to 8179 A. The system should be present in S-type stars. Our observed isotope shift for the v = 2 sequence agrees with calculations. 16 bands of the γ-system ($A^3\phi$ - $X'^3\Delta$) have been analysed up to v' = 5, v'' = 6. When vibrational and rotational constants were calculated additional constants for higher order terms had to be included. The infrared spectrum of ZrO shows several bands between 8786 cm^{-1} and 10309 cm^{-1}. Identifications are under way. The well known 9290 A band consists probably of three Q branches of a predicted triplet system. The 8192 A band has been resolved into three branches belonging to a doublet system, presumably of ZrO^+. A laboratory source enhancing the abundance of ZrO^+ is being developed.

2. Lifetimes and Absolute Transition Probabilities

TiO: A tunable dye laser has been used to measure the lifetime of the $C^1\phi$ state. Our results on the intercombination transitions ($C^3\Delta_3$ - $a^1\Delta_3$) agree with those of Broida and Linton, but we have problems to explain the anomalously weak P-line. Further intercombination emissions are being sought. For the α-system of TiO ($C^3\Delta_3$ - $X^3\Delta_3$) the radiative lifetime of two rotational levels of v' = 2 ($C^3\Delta_3$) has been measured by laser-induced fluorescence and delayed coincidence. The results are τ = 28.21±0.15 nsec for J' = 17, and τ = 29.74±0.86 nsec for J' = 87. Ar - TiO collision cross-sections for the two levels have been determined to differ by 30%.
ZrO: We have recently (May 1978) collected data on the lifetime of the $B^3\Pi$ state using observations on the $\beta(B^3\Pi - X^3\Delta)$ system.

D. *From the Centre for Astrophysics, Harvard College Observatory*
(Reported by W.H. Parkinson and J.L. Kohl)

The Atomic and Molecular Physics Division of the Harvard-Smithsonian Center for Astrophysics is engaged in quantitative studies of basic atomic and molecular processes having applications to astrophysical problems. A variety of experimental techniques and instruments are used to study atomic autoionization, photoionization, spectral lines broadening and radiative bound state transitions. A new Ion-Beam Facility was recently built to study the interaction of multiple charged ions with other particles and radiation fields, and the Division recently acquired a 6.6 meter evacuable spectrograph for quantitative measurements of molecular spectra and structure. The experimental work is closely associated with theoretical studies of atoms and molecules by the Center's Theoretical Atomic and Molecular Physics Group (208,209,210,211,212).

E. *From the Cavendish Laboratory, University of Cambridge*
(Reported by A.H. Cook)

Molecular spectroscopy in the Laboratory Astrophysics group is undertaken with the aim of contributing to the understanding of maser action in astrophysics. A research student (J. Viney) has observed the pure rotation spectrum of OH using a Fourier transform far-infra-red spectrometer at the National Physical Laboratory and has detected transitions between the $^2\Pi_{3/2}$ and $^2\Pi_{1/2}$ series as well as transitions within each series. Mr. Viney has also used the synchrotron source and associated far ultraviolet spectrograph at Bonn to look for the ultraviolet spectra of molecules of astrophysical interest. He has seen spectra almost certainly to be attributed to Rydberg series of SiO (a molecule which shows maser action) and he has observed a sequence of broad bands very probably to be attributed to OH. These observations lie in the range 70-100 nm.

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F. *From the Centre for Research in Experimental Space Science, York University, Toronto*
(Reported by R.W. Nicholls)

The multifaceted experimental and theoretical research programme to provide absolute transition probability data and structure constants for astrophysical molecules continues, see also (4). Recommendations have also been made for consistent definitions of transition moments and line intensity factors for molecular spectra (15). A programme of high resolution shock tube spectroscopy and radiometry continues to provide transition probability data on C_2 (213), ScO (214), TiO, WO and ZrO. The same equipment provides high resolution spectra for band analyses of YO (215), WO and ZrO. High resolution photoelectric studies of CN have been interpreted by the method of synthetic spectra to provide transition probability data for the Violet (216) and Red Systems. Medium resolution (217) and high resolution measurements have been made of the absolute absorption coefficients of the ClO ($A^2\Pi - X^2\Pi$) bands. Realistic computer syntheses of Cometary spectra have been compared with observed spectra to diagnose physical conditions in Comets (218). High resolution computer syntheses have also been made of atmospheric transmission (219,220). The same facility has been used to assess CO_2 line position data (221). Theoretical studies have continued on molecular transition probabilities. Band strengths of the IR vibration-rotation bands of ClO have been calculated (222) and model studies have been made on the r-centroid approximation (223) and of photodissociation processes.

G. *Other Laboratories*

Lindgren has provided a set of extensive annual reports on the large research programme on diatomic molecular spectroscopy at Stockholm, some of which is devoted to astrophysical molecules and is referenced above. Leach provided reprints from an extensive research programme on diatomics and polyatomics in his Laboratoire de Photophysique (Paris), some of which are referenced above. Judge provided an extensive reference and reprint list of the research programme on vacuum UV photo-fluorescence studies at the University of Southern California.

REFERENCES

1. Phillips, J.G., Davis, S.P.: "Berkeley Newsletter", Departments of Astronomy and Physics, University of California, Berkeley, Calif.
2. Herzberg, G., Huber, K.P.: 1978, "Constants of Diatomic Molecules", Van Nostrand and Reinhold, New York.
3. Hsu, D.K., Smith, W.H.: 1977, Spect. Letts. 10, p. 181.
4. Nicholls, R.W.: 1977, Ann. Rev. Astron. Astrophys. 15, p. 197.
5. Lofthus, A., Krupenie, P.H.: 1977, J. Phys. Chem. Ref. Data 6, p. 113.
6. Pearse, R.W.B., Gaydon, A.G.: 1976, "Identification of Molecular Spectra", 4th Edn. Revised, Chapman and Hall, London.
7. Kopp, I., Jansson, K., Rydh, B.: 1977, "Table of Band Features of Diatomic Molecules in Wavelength Order", Institute of Physics, University of Stockholm (International Tables of Constants, Paris).
8. Hsu, D.K., Monts, D.L., Zare, R.N.: 1978, "Spectral Atlas of NO_2 5530-6480A", Academic Press, New York.
9. Park, J.H.: 1977, "Atlas of IR Absorption Lines", NASA Contractor Report 2925.
10. Nordstrom, R.J., Shaw, J.H., Skinner, W.R., Calvert, J.G., Chan, W.H., Uselman, W.M.: 1976, "A Comparison of High Resolution Observed and Computed Air Spectra between 700 and 2300 cm^{-1}", RF4221 Tech. Rept. Ohio State Univ. Research Foundation.
11. Roney, P.L., Findlay, F.D., Buijs, H.L., Cann, M.W.P., Nicholls, R.W.: 1978, Applied Optics 17, p. 2599.
12. Rothman, L.S., Benedict, W.S.: 1978, Applied Optics 17, p. 2605.
13. Mulliken, R.S., Ermler, W.C.: 1977, "Diatomic Molecules, Results of ab initio

Calculations", Academic Press, New York.
14. Bunker, P.R.: 1978, "Molecular Symmetry and Spectroscopy", Academic Press, New York.
15. Whiting, E.E., Schadee, A., Tatum, J.B., Hougen, J.T., Nicholls, R.W.: 1978, J. Chem. Phys., submitted.
16. Ames, S., Huebner, W.F.: 1977, "Emission Cross Sections for Rotational Transitions of Astrophysical Interest", Los Alamos Scientific Laboratory Report LA6366.
17. Kuriyan, M., Pritchard, H.O.: 1976, Can. J. Chem. 54, p. 1865.
18. Kuriyan, M., Pritchard, H.O.: 1977, Can. J. Chem. 55, p. 3420.
19. Schadee, A.: 1978, J. Quant. Spectr. Rad. Transf. 19, p. 517.
20. Hefferlin, R.: 1978, J. Quant. Spectr. Rad. Transf. 19, p. 335.
21. Wolniewicz, L., Dressler, K.: 1977, J. Mol. Spectrosc. 67, p. 416.
22. Ledbetter, J.W., Dressler, K.: 1976, J. Mol. Spectrosc. 63, p. 370.
23. Dressler, K.: 1976, J. Chem. Phys. 64, p. 3493.
24. Chojnicki, A.H.: 1978, Thesis, Oxford.
25. Pouilly, B., Schamps, J., Lumley, D.J.W., Barrow, R.F.: 1978, J. Phys. B: At. Mol. Phys. 11, p. 2289.
26. Kotlar, A.J.: 1978, Thesis, M.I.T.
27. Linton, C., Broida, H.P.: 1977, J. Mol. Spectrosc. 64, p. 382.
28. Linton, C., Broida, H.P.: 1977, J. Mol. Spectrosc. 64, p. 389.
29. Shanker, R., Linton, C., Verma, R.D.: 1976, J. Mol. Spectrosc. 60, p. 197.
30. Linton, C., Cappelle, G.A.: 1977, J. Mol. Spectrosc. 66, p. 62.
31. Linton, C.: 1978, J. Mol. Spectrosc. 69, p. 351.
32. Bartoe, J.D.F., Brueckner, G.E., Sandlin, G.D., Van Hoosier, M.E., Jordan, C.: 1978, Astrophys. J. Letts., in press.
33. Jordan, C., Brueckner, G.E., Bartoe, J.D.F., Sandlin, G.D., Van Hoosier, M.E.: 1977, Nature 270, p. 326.
34. Graham, W.R.M., Lew, H.: 1978, Can. J. Phys. 56, p. 85.
35. Orth, F.B., Brown, C.M., Ginter, M.L.: 1978, J. Mol. Spectrosc. 69, p. 53.
36. Brown, C.M., Ginter, M.L.: 1978, J. Mol. Spectrosc. 69, p. 25.
37. Dick, K.A., Benesch, W., Crosswhite, H.M., Tilford, S.G., Gottscho, R.A. Field, R.W.: 1978, J. Mol. Spectrosc. 69, p. 95.
38. Beiting, E.J., Jones, C.C., Benesch, W.: 1978, J. Mol. Spectrosc. 70, p. 108.
39. Benesch, W., Jones, C.C., Beiting, E.J., Feldman, P.D.: 1978, J. Opt. Soc. Am. 68, p. 432.
40. Jones, C.C., Benesch, W., Beiting, E.J.: 1978, J. Mol. Spectrosc. 70, p. 95.
41. Balfour, W.J., Lindgren, B.: 1978, Can. J. Phys., in press.
42. Nordh, H.L., Lindgren, B., Wing, R.F.: 1977, Astron. Astrophys. 56, p. 1.
43. McKellar, A.R.W., Goetz, W., Ramsay, D.A.: 1976, Astrophys. J. 207, p. 663.
44. Coxon, J.A., Ramsay, D.A.: 1976, Can. J. Phys. 54, p. 1034.
45. Lin, C.L., Gutman, W.M., Shaw, J.H., Uselman, W.M., Calvert, J.G.: 1978, Applied Optics 17, p. 993.
46. Shaw, J.H., Lin, C.L.: 1978, "The Application of the IBM Library Programme BMDP3R (Non-Linear Least Squares Fit) to Retrieving Parameters of Spectral Lines from Absorption Spectra", RF Prog. 700279 Interim Report, Ohio State Univ. Research Foundation.
47. Cossart, D., Horani, M., Rostas, J.: 1977, J. Mol. Spectrosc. 67, p. 283.
48. Schadee, A.: 1978, J. Quant. Spectr. Rad. Transf. 19, p. 451.
49. Erman, P.: 1975, Phys. Script. 11, p. 65.
50. Brzozowski, J., Elander, N., Erman, P., Lyyra, M.: 1974, Astrophys. J. 193, p. 741.
51. Brzozowski, J., Elander, N., Erman, P., Lyyra, M.: 1974, Phys. Script. 10, p. 241.
52. Brzozowski, J., Erman, P., Lew, H.: 1975, Chem. Phys. Letts. 34, p. 267.
53. Smith, W.H., Brzozowski, J., Erman, P.: 1976, J. Chem. Phys. 64, p. 4628.
54. Brzozowski, J., Bunker, P., Elander, N., Erman, P.: 1976, Astrophys. J. 207, p. 414.
55. Callear, A.B., Erman, P., Kurepa, J.: 1976, Chem. Phys. Letts. 44, p. 599.

56. Curtis, L., Engman, B., Erman, P.: 1976, Phys. Script. 13, p. 270.
57. Erman, P.: 1976, Phys. Script. 14, p. 51.
58. Brzozowski, J., Erman, P., Lyyra, M.: 1976, Phys. Script. 14, p. 290.
59. Curtis, L.J., Erman, P.: 1977, J. Opt. Soc. Am. 67, p. 1218.
60. Erman, P.: 1977, Astrophys. J. Letts. 213, p. L89.
61. Erman, P.: 1977, Phys. Script. 16, p. 60.
62. Brzozowski, J., Erman, P., Lyyra, M.: 1978, Phys. Script. 17, p. 507.
63. Duric, N., Erman, P., Larsson, M.: 1978, Phys. Script. 18, p. 39.
64. Carlson, T.A., Duric, N., Erman, P., Larsson, M.: 1978, Z. Physik A287, p. 123.
65. Carlson, T.A., Duric, N., Erman, P., Larsson, M.: 1978, J. Phys. B: At. Mol. Phys. 11, p. 3667.
66. Huie, R.E., Long, N.J.T., Thrush, B.A.: 1978, Chem. Phys. Letts. 55, p. 404.
67. Llewellyn, E.J., Long, B.H.: 1978, Can. J. Phys. 56, p. 581.
68. Llewellyn, E.J., Solheim, B.H.: 1978, Planet. Sp. Sci. 26, p. 533.
69. Llewellyn, E.J., Long, B.H., Solheim, B.H.: 1978, Planet. Sp. Sci. 26, p. 525.
70. Leach, S., Velghe, M.: 1976, J. Quant. Spectr. Rad. Transf. 16, p. 861.
71. Steele, R.E., Linton, C.: 1978, J. Mol. Spectrosc. 69, p. 66.
72. Feinberg, J., Davis, S.P.: 1977, J. Mol. Spectrosc. 65, p. 264.
73. Feinberg, J., Davis, S.P.: 1978, J. Mol. Spectrosc. 69, p. 445.
74. Price, M.L., Sulzmann, K.G.P., Penner, S.S.: 1974, J. Quant. Spectr. Rad. Transf. 14, p. 1273.
75. Sulzmann, K.G.P.: 1975, J. Quant. Spectr. Rad. Transf. 15, p. 313.
76. Heffington, W.M., Parks, G.E., Sulzmann, K.G.P., Penner, S.S.: 1976, J. Quant. Spectr. Rad. Transf. 16, p. 839.
77. Sulzmann, K.G.P.: 1974, J. Quant. Spectr. Rad. Transf. 14, p. 413.
78. Sulzmann, K.G.P.: 1974, J. Quant. Spectr. Rad. Transf. 14, p. 1157.
79. Tilford, S.G., Benesch, W.M.: 1976, J. Chem. Phys. 64, p. 3370.
80. Marr, G.V., Woodruff, P.R.: 1976, J. Phys. B: At. Mol. Phys. 9, p. L377.
81. Woodruff, P.R., Marr, G.V.: 1977, Proc. Roy. Soc. A358, p. 87.
82. Gardner, J.L., Samson, J.A.: 1976, J. Elect. Spect. Rel. Phenom. 8, p. 123.
83. Samson, J.A.R., Haddad, G.N., Gardner, J.L.: 1977, J. Phys. B: At. Mol. Phys. 10, p. 1749.
84. Samson, J.A.R., Gardner, J.L., Haddad, G.N.: 1977, J. Elect. Spect. Rel. Phenom. 12, p. 281.
85. Gardner, J.L., Samson, J.A.R.: 1978, J. Elect. Spect. Rel. Phenom. 13, p. 7.
86. Samson, J.A.R., Kemeny, P.C., Haddad, G.N.: 1977, Chem. Phys. Letts. 51, p. 75.
87. Samson, J.A.R., Gardner, J.L.: 1976, J. Elect. Spect. Rel. Phenom. 8, p. 35.
88. Samson, J.A.R., Gardner, J.L.: 1977, J. Chem. Phys. 67, p. 755.
89. Gattinger, R.L.: 1976, Planet. Sp. Sci. 24, p. 999.
90. Gattinger, R.L., Vallance Jones, A.: 1976, J. Geophys. Res. 81, p. 4789.
91. Jones, A.V., Gattinger, R.L.: 1976, Can. J. Phys. 54, p. 2128.
92. Chang, Y.S., Shaw, J.H.: 1977, J. Quant. Spectr. Rad. Transf. 18, p. 491.
93. Chang, Y.S., Shaw, J.H., Calvert, J.G., Uselman, W.M.: 1977, J. Quant. Spectr. Rad. Transf. 18, p. 589.
94. Lewis, B.R., Carver, J.H., Hobbs, T.I., McCoy, D.G., Giess, H.P.F.: 1977, "Experimentally Determined Oscillator Strengths and Linewidths for the Schumann-Runge Band System and Molecular Oxygen 60-140 Bands", University of Adelaide, Department of Physics (ADP149 Report 149).
95. Park, C., Arnold, J.O.: 1978, J. Quant. Spectr. Rad. Transf. 19, p. 1
96. Smith, P.L., Huber, M.C.E., Parkinson, W.H.: 1976, Phys. Rev. A13, p. 1422.
97. Hartmann, G., Johnson, P.C.: 1978, J. Phys. B: At. Mol. Phys. 11, p. 1597.
98. Provorov, A.C., Stoicheff, B.P., Wallace, S.: 1977, J. Chem. Phys. 67, p. 5393.
99. Langhoff, S.R., Arnold, J.O.: 1978, J. Chem. Phys., in press.
100. Arnold, J.O., Langhoff, S.R.: 1978, J. Quant. Spectr. Rad. Transf. 19, p. 461.
101. Jaffe, R.L., Langhoff, S.R.: 1978, J. Chem. Phys. 68, p. 1638.
102. Rumble, J.R., Sims, J.S., Purdy, D.R.: 1977, J. Phys. B: At. Mol. Phys. 10, p. 2553.
103. Watson, D.K., Steward, R.F., Dalgarno, A.: 1976, J. Chem. Phys. 64, p. 4995.
104. Cerjan, C.J., Docken, K.K., Dalgarno, A.: 1976, Chem. Phys. Letts. 38, p. 401.

105. Watson, D.K., Steward, R.F., Dalgarno, A.: 1976, Mol. Phys. 32, p. 1661.
106. Watson, D.K., Cerjan, C.J., Guberman, S., Dalgarno, A.: 1977, Chem. Phys. Letts. 50, p. 181.
107. Steward, R.F., Watson, D.K., Dalgarno, A.: 1976, J. Chem. Phys. 65, p. 2104.
108. Turner, J., Kirby-Docken, K., Dalgarno, A.: 1977, Astrophys. J. Suppl. 35, p. 281.
109. Johns, J.W.C., Ramsay, D.A., Ross, S.C.: 1976, Can. J. Phys. 54, p. 1804.
110. Birss, F.W., Braund, D.B., Cole, A.R.H., Engleman, R., Green, A.A., Japar, S.M., Nanes, R., Orr, B.J., Ramsay, D.A., Szyszka, J.: 1977, Can. J. Phys. 55, p. 390.
111. Hardwick, J.L., Ramsay, D.A.: 1977, Chem. Phys. Letts. 48, p. 399.
112. Birss, F.W., Ramsay, D.A., Till, S.M.: 1978, Chem. Phys. Letts. 53, p. 14.
113. Vervloet, M., Merienne-Lafore, M.F., Ramsay, D.A.: 1978, Chem. Phys. Letts. 57, p.5.
114. Kroto, H.W., Kirby, C., Walton, D.R.M., Avery, L.W., Broten, N.W., MacLeod, J.M., Oka, T.: 1978, Astrophys. J. Letts. 219, p. L133.
115. Broten, N.W., MacLeod, J.M., Oka, T., Avery, L.W., Brooks, J.W., McGee, R.X., Newton, L.M.: 1976, Astrophys. J. Letts. 209, p. L143.
116. Avery, L.W., Broten, N.W., MacLeod, J.M., Oka, T., Kroto, H.W.: 1976, Astrophys. J. Letts. 205, p. L173.
117. Oka, T.: 1976, Molecular Spectra Modern Research 2, p. 229.
118. Laughton, D., Freund, S.M., Oka, T.: 1976, J. Mol. Spectrosc. 62, p. 263.
119. Orr, B.J., Oka, T.: 1977, J. Mol. Spectrosc. 66, p. 302.
120. Freund, S.M., Oka, T.: 1976, Phys. Rev. A 13, p. 2178.
121. Landsberg, B.M., Merer, A.J., Oka, T.: 1977, J. Mol. Spectrosc. 67, p. 459.
122. Retallack, L.J., Lees, R.M.: 1976, J. Chem. Phys. 65, p. 3793.
123. Lees, R.M.: 1978, J. Mol. Spectrosc. 69, p. 225.
124. Retallack, L.J., Lees, R.M., Van der Linde, J.: 1976, J. Mol. Spectrosc. 63, p. 527
125. Lees, R.M., Retallack, L.J.: 1976, Chem. Phys. Letts. 41, p. 583.
126. Gerry, M.C.L., Lees, R.M., Winnewisser, G.: 1976, J. Mol. Spectrosc. 61, p. 231.
127. Ozier, I., Lees, R.M., Gerry, M.C.L.: 1976, J. Chem. Phys. 65, p. 1795.
128. Ozier, I., Lees, R.M., Gerry, M.C.L.: 1976, Can J. Phys. 54, p. 1094.
129. Winnewisser, G., Hocking, W.H., Gerry, M.C.L.: 1976, J. Phys. Chem. Ref. Data 5, p. 79.
130. Kagann, R.H., Ozier, I., Gerry, M.C.L.: 1976, J. Chem. Phys. 64, p. 3487.
131. Creswell, R.A., Winnewisser, G., Gerry, M.C.L.: 1977, J. Mol. Spectrosc. 65, p. 420.
132. Hocking, W.H., Gerry, M.C.L.: 1976, J. Mol. Spectrosc. 59, p. 338.
133. Davis, R.W., Gerry, M.C.L.: 1976, J. Mol. Spectrosc. 59, p. 407.
134. Yamada, K., Winnewisser, M., Winnewisser, G., Szalanski, L.B., Gerry, M.C.L.: 1977, J. Mol. Spectrosc. 64, p. 401.
135. Lutz, B.L., Owen, T., Cess, R.D.: 1976, Astrophys. J. 203, p. 541.
136. Danehy, R.G., Lutz, B.L., Owen, T., Scattergood, T.W., Goetz, W.: 1977, Astrophys. J. Letts. 213, p. L139.
137. Lutz, B.: 1978, J. Mol. Spectrosc., in press.
138. Lutz, B.: 1978, Astrophys. J., in press.
139. Leach, S.: 1976, "Optical Spectroscopy of Molecular Ions", in "Spectroscopy of the Excited State", Ed. B. di Bartolo, p. 369, Plenum, New York.
140. Gauyacq, D., Horani, M., Leach, S., Rostas, J.: 1975, Can. J. Phys. 53, p. 2040.
141. Balfour, W.J.: 1976, Can. J. Phys. 54, p. 1969.
142. Frost, D.C., Lee, S.T., McDowell, C.A., Westwood, N.P.C.: 1976, J. Chem. Phys. 64, p. 4719.
143. Frost, D.C., Lee, S.T., McDowell, C.A., Westwood, N.P.C.: 1977, J. Elect. Spect. Rel. Phenom. 12, p. 95.
144. Bolman, P.S.H., Brown, J.M., Carrington, A., Kopp, I., Ramsay, D.A.: 1975, Proc. Roy. Soc. A343, p. 17.

145. Gewurtz, S., Lew, H., Flainek, P.: 1975, Can. J. Phys. 53, p. 1097.
146. Alberti, F., Douglas, A.E.: 1975, Can. J. Phys. 53, p. 1179.
147. Kroll, M.: 1975, J. Chem. Phys. 63, p. 319.
148. Kroll, M.: 1975, J. Chem. Phys. 63, p. 1803.
149. Brzozowski, J., Erman, P., Lew, H.: 1975, Chem. Phys. Lett. 34, p. 267.
150. Coxon, J.A., Ramsay, D.A., Setser, D.W.: 1975, Can. J. Phys. 53, p. 1587.
151. Douglas, A.E., Hoy, A.R.: 1975, Can. J. Phys. 53, p. 1965.
152. Kreiner, W.A., Oka, T.: 1975, Can. J. Phys. 53, p. 2000.
153. Hoy, A.R., Johns, J.W.C., McKellar, A.R.W.: 1975, Can. J. Phys. 53, p. 2029.
154. Colin, R., De Greef, D.: 1975, Can. J. Phys. 53, p. 2142.
155. Johns, J.W.C., Kreiner, W.A., Susskind, J.: 1976, J. Mol. Spectrosc. 60, p. 400
156. Dabrowski, I., Herzberg, G.: 1976, Can. J. Phys. 54, p. 525.
157. Coxon, J.A., Ramsay, D.A.: 1976, Can. J. Phys. 54, p. 1034.
158. Bunker, P.R.: 1976, J. Mol. Spectrosc. 61, p. 319.
159. Colbourn, E.A., Dagenais, M., Douglas, A.E., Raymonda, J.W.: 1976, Can. J. Phys. 54, p. 1343.
160. Freund, S.M., Oka, T.: 1976, Phys. Rev. A 13, p. 2178.
161. McKellar, A.R.W., Goetz, W., Ramsay, D.A.: 1976, Astrophys. J. 207, p. 663.
162. Johns, J.W.C., Ramsay, D.A., Ross, S.C.: 1976, Can. J. Phys. 54, p. 1804.
163. Lew, H.: 1976, Can. J. Phys. 54, p. 2028.
164. Miescher, E., Alberti, F.: 1976, J. Phys. Chem. Ref. Data 5, p. 309.
165. Freedman, P.A.: 1976, Chem. Phys. Lett. 44, p. 605.
166. Miescher, E., Huber, K.P.: 1976, International Review of Science, Physical Chemistry (2), Vol. 3, p. 37, Butterworths, London.
167. Johns, J.W.C., McKellar, A.R.W.: 1977, J. Chem. Phys. 66, p. 1217.
168. Johns, J.W.C., McKellar, A.R.W.: 1977, J. Mol. Spectrosc. 64, p. 327.
169. Colbourn, E.A., Douglas, A.E.: 1977, J. Mol. Spectrosc. 65, p. 332.
170. Dabrowski, I., Herzberg, G.: 1977, Trans. N.Y. Acad. Sci. 38, II, p. 14.
171. Hardwick, J.L., Ramsay, D.A.: 1977, Chem. Phys. Lett. 48, p. 399.
172. Danehy, R.G., Lutz, B.L., Owen, T., Scattergood, T.W., Goetz, W.: 1977, Astrophys. J. Letts. 213, p. L139.
173. Allegrini, M., Johns, J.W.C., McKellar, A.R.W.: 1977, J. Mol. Spectrosc. 66, p. 69.
174. Hardwick, J.L.: 1977, J. Mol. Spectrosc. 66, p. 248.
175. Orr, B.J., Oka, T.: 1977, J. Mol. Spectrosc. 66, p. 302.
176. Dale, R.M., Johns, J.W.C., McKellar, A.R.W., Riggin, M.: 1977, J. Mol. Spectrosc. 67, p. 440.
177. Landsberg, B.M., Merer, A.J., Oka, T.: 1977, J. Mol. Spectrosc. 67, p. 459.
178. Allegrini, M., Johns, J.W.C., McKellar, A.R.W.: 1977, J. Mol. Spectrosc. 67, p. 476.
179. Johns, J.W.C., McKellar, A.R.W., Riggin, M.: 1977, J. Chem. Phys. 67, p. 2427.
180. Tipping, R.H., Poll, J.D., McKellar, A.R.W.: 1978, Can. J. Phys. 56, p. 75.
181. Johns, J.W.C., Riggin, M., McKellar, A.R.W.: 1978, J. Chem. Phys., in press.
182. Reid, J., McKellar, A.R.W.: 1978, Phys. Rev. A, in press.
183. Allegrini, M., Johns, J.W.C., McKellar, A.R.W.: 1978, Can. J. Phys., in press.
184. Dabrowski, I., Herzberg, G.: 1978, J. Mol. Spectrosc., in press.
185. Bauder, A., Lovas, F.J., Johnson, D.R.: 1976, J. Phys. Chem. Ref. Data 5, p. 53.
186. Winnewisser, G., Hocking, W.H., Gerry, M.C.L.: 1976, J. Phys. Chem. Ref. Data 5, p. 79.
187. Tiemann, E.: 1976, J. Phys. Chem. Ref. Data 5, p. 1147.
188. Beaudet, R.A., Poynter, R.L.: 1978, J. Phys. Chem. Ref. Data 7, p. 311.
189. Lafferty, W.J., Lovas, F.J.: 1978, J. Phys. Chem. Ref. Data 7, p. 441.
190. Gerry, M.C.L., Yamada, K., Winnewisser, G.: 1978, J. Phys. Chem. Ref. Data, in press.
191. Bauer, A., Boucher, D., Burie, J., Demaison, J., Dubrulle, A.: Université de Sciences et Techniques de Lille, work in progress.
192. Willemot, E., Dangoisse, D., Monnanteuil, N., Bellet, J.: Université des Sciences et Techniques de Lille, work in progress.

193. Bauder, A.: Swiss Federal Institute of Technology, Zurich, work in progress.
194. Lovas, F.J. (NBS), Dreizler, H., Lutz, H.: University of Kiel, work in progress.
195. Lovas, F.J., Snyder, L.E. (University of Illinois), Johnson, D.R. (NBS), work in progress.
196. Lovas, F.J.: 1978, J. Phys. Chem. Ref. Data 7 (4).
197. Miescher, E., Alberti, F.: 1976, J. Phys. Chem. Ref. Data 5, p. 309.
198. Lofthus, A., Krupenie, P.H.: 1977, J. Phys. Chem. Ref. Data 6, p. 113.
199. Pearson, R. Jr., Lovas, F.J.: 1977, J. Chem. Phys. 66, p. 4149.
200. Johnson, D.R., Lovas, F.J., Gottlieb, C.A., Gottlieb, E.W., Litvak, M.M., Guelin, M., Thaddeus, P.: 1977, Astrophys. J. 218, p. 370.
201. Johnson, D.R., Suenram, R.D., Lafferty, W.J.: 1976, Astrophys. J. 208, p. 245.
202. Lovas, F.J., Suenram, R.D.: work in progress.
203. Hougen, J.T., Mucha, J.A., Jenning, D.A., Evenson, K.M.: J. Mol. Spectrosc., to be published.
204. Todd, T.R.: 1977, J. Mol. Spectrosc. 66, p. 162.
205. Todd, T.R., Olson, W.B.: 1978, J. Mol. Spectrosc., submitted.
206. Maki, A.G., Sams, R.L.: in preparation.
207. Jacox, M.E.: 1977, J. Mol. Spectrosc. 66, p. 272.
208. Tanaka, Y., Yoshino, K., Freeman, D.E.: 1975, J. Chem. Phys. 62, p. 4484.
209. Yoshino, K., Ogawa, M., Tanaka, Y.: 1976, J. Mol. Spectrosc. 61, p. 403.
210. Freeman, D.E., Yoshino, K., Tanaka, Y.: 1977, J. Chem. Phys. 67, p. 3462.
211. Yoshino, K., Tanaka, Y.: 1977, J. Mol. Spectrosc. 66, p. 219.
212. Parkinson, W.H.: 1978, Astrophys. J. Letts., in press.
213. Cooper, D.M., Nicholls, R.W.: 1976, Spect. Letts. 9, p. 139.
214. Shin, J.B., Nicholls, R.W.: 1978, Proc. 11th International Symposium on Shock Tubes and Waves, Seattle 1977, Eds. Ahlborn, Hertzberg and Russell, p. 140, Univ. of Washington Press, Seattle.
215. Shin, J.B., Nicholls, R.W.: 1977, Spect. Letts. 10, p. 923.
216. Danylewych, L.L., Nicholls, R.W.: 1978, Proc. Roy. Soc. A 360, p. 557.
217. Mandelman, M., Nicholls, R.W.: 1977, J. Quant. Spectr. Rad. Transf. 17, p. 483.
218. Danylewych, L.L., Nicholls, R.W., Neff, J.S., Tatum, J.B.: 1978, Icarus 35, p. 112.
219. Cann, M.W.P., Nicholls, R.W., Evans, W.F.J., McEwen, D.J.: 1976, Atmosphere 14, p. 205.
220. Cann, M.W.P., Nicholls, R.W., Evans, W.F.J., Kohl, J.L., Kurucz, R., Parkinson, W.H., Reeves, E.M.: 1978, Applied Optics, in press.
221. Roney, P.L., Findlay, F.D., Buijs, H.L., Cann, M.W.P., Nicholls, R.W.: 1978, Applied Optics 17, p. 2599.
222. Langhoff, S.R., Dix, J.P., Arnold, J.O., Nicholls, R.W., Danylewych, L.L.: 1977, J. Chem. Phys. 67, p. 4306.
223. Nicholls, R.W.: 1976, Spect. Letts. 9, p. 23.

R.W. NICHOLLS
Chairman of the Working Group

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