## J. F. Ogilvie scientific and educational publications

## A theses and books

Infrared Spectra of Reactive Species (supervisor K. B. Harvey)
M.Sc. thesis, University of British Columbia, Canada, 1961 August
Spectroscopic Studies of Trapped Radicals (supervisor R. G. W. Norrish, F.R.S., Nobel)
Ph.D. thesis, University of Cambridge, England UK, 1965 October
The Vibrational and Rotational Spectrometry of Diatomic Molecules
Academic Press, London, UK, 1998
Mathematics for Chemistry with Symbolic Computation
Maplesoft, Waterloo, Canada, 2005, first edition
edition 6, 2021 August, https://www.maplesoft.com/applications/view.aspx?SID=154267
Models, Mysteries and Magic of Molecules, editors J. C. A. Boeyens and J. F. Ogilvie
Springer Science, Dordrecht, Netherlands, 2008
Fourier Transforms for Chemistry
Maplesoft, Waterloo, Canada, 2021
https://www.maplesoft.com/applications/view.aspx?SID=154672
Quantum Mechanics for Chemistry
Maplesoft, Waterloo, Canada, 2021
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## **B** original papers in scientific research

1	Infrared absorption of methanal at low temperatures
	Canadian Journal of Chemistry 40 (1962) 85-91 (with K. B. Harvey)
2	Infrared absorption of the hydroxyl radical.
	<i>Nature</i> , <b>204</b> (1964) 572.
3	Extension of the grating range of the SP100 spectrometer
	Journal of Scientific Instruments 42 (1965) 352
4	Structure and photochemistry of methanal azine
	Chemical Communications (1965) 359-360
5	Electronic absorption spectrum of the H <sub>3</sub> CO radical
	<i>Nature</i> , <b>208</b> (1965) 1315.
6	Spectroscopic studies of the photodecomposition of silyl azide in argon matrices near 4 K: detection
	of iminosilicon, HNSi
	Chemical Communications (1966), 364-365 (with S. Cradock)
7	Cryogenics, infrared spectrometry and photochemistry
	Unicam Spectrovision, No. 16, (1966) 1-5
8	The vibrational fundamentals and structures of triatomic radicals formed by photolytic reactions of
	hydrogen atoms
	Spectrochimica Acta, <b>23A</b> (1967) 737-750
9	Electronic absorption spectra of methanal azine and the methyleniminyl free radical
	Journal of Chemical Physics 48 (1968) 2248-2256 (with D. G. Horne)
1(	) Photodecomposition of trimethylsilyl azide in solid argon

*Nature*, **218** (1968) 1248-1249

- 11 On the purported infrared absorption at 21 μm of CO adsorbed on silica-supported Pt Journal of Physical Chemistry 72 (1968) 2688
- 12 Vibrational absorption of the diazomethyl radical Canadian Journal of Chemistry **46** (1968) 2472-2474
- 13 Structural deductions from vibronic spectra of ethene and ethene-d<sub>4</sub> Journal of Chemical Physics **49** (1968) 474-475
- 14 A spectroscopic study of the photodecomposition of diazomethane *Photochemistry and Photobiology* **9** (1969) 65-90
- 15 Spectroscopic investigation of diazomethane isomers Journal of Molecular Structure **3** (1969) 513-516
- 16 Spectral data and bonding in compounds of silicon and germanium with nitrogen *Transactions of the Faraday Society* **65** (1969) 2602-2606 (with M. J. Newlands)
- 17 Applications of bonding in metallo-organic compounds to nitrogen fixation Discussions of the Faraday Society **47** (1969) 203 (with M. J. Newlands)
- 18 Structures of electronically excited molecules Journal of Molecular Structure **5** (1970) 157-177
- 19 Photochemical production of acetylmanganese carbonyls in an argon matrix at 17 K *Chemical Communications* (1970), 323-324
- 20 Vibration-rotational bands of butadiene-1,3: evidence for Coriolis coupling Journal of Molecular Spectroscopy **35** (1970) 332-334 (with K. C. Cole)
- 21 The dihydrogen-dioxygen second explosion limit Journal of Chemical Education **48** (1971) 342-344
- 22 Vibrational spectra and conformation of methanal azine Spectrochimica Acta, **27A** (1971) 877-895 (with K. C. Cole)
- 23 Hydrocarbon complexes of iron carbonyls formed photochemically in argon matrices at 17K *Canadian Journal of Chemistry* **49** (1971) 343 (with M. J. Newlands)
- 24 Semi-experimental determination of a repulsive potential-energy curve for hydrogen iodide *Transactions of the Faraday Society* **67** (1971) 2205-2215
- 25 Kinetic energy of hydrogen atoms from photolysed hydrogen iodide Faraday Discussions of the Chemical Society **53** (1972) 153 (with R. H. Tipping)
- 26 Intense vibrational absorption spectra of trapped triatomic radicals *Nature*, **243** (1973) 210-212
- 27 Vibrational assignments for methyl nitrite rotamers Chemical Communications (1973), 450-451
- 28 Harmonic force fields and mean amplitudes of vibration for some molecules containing nitrogen: methanal azine
  - Journal of Molecular Structure 18 (1973) 285-293 (with S. J. Cyvin and B. N. Cyvin)
- 29 Infrared absorption of hydrogen atoms in solid argon and krypton Journal of Chemical Physics **59** (1973) 3871
- 30 Dunham potential-energy parameters of weakly bound homonuclear molecules Faraday Discussions of the Chemical Society **55** (1973) 189-190 (with R. W. Davis)
- 31 Electronic transitions in methanal azine and related molecules *Canadian Journal of Spectroscopy* **19** (1974) 89-95
- 32 Force parameters of triatomic molecules and radicals Canadian Journal of Spectroscopy **19** (1974) 171-177
- 33 Photo-oxidation of iodomethane in solid argon Canadian Journal of Chemistry 53 (1975) 269-275 (with V. R. Salares and M. J. Newlands)
- 34 Photoelectron spectra of methanal azine Canadian Journal of Spectroscopy **20** (1975) 162-166 (with K. C. Cole)

35 Structures of triatomic radicals HCO, HNO and HOO Journal of Molecular Structure 31 (1976) 407-410 36 Dunham potential-energy coefficients of the hydrogen halides and carbon oxide Journal of Molecular Spectroscopy 61 (1976) 332-336 (with D. Koo) 37 Planarity of the methyl radical Spectroscopy Letters 9 (1976) 203-210 38 Calculated molecular orientational disorder in anthracene crystals Journal of the Chemical Society Faraday Transactions II, 72 (1976) 1602-1612 (with D. P. Craig and P. A. Reynolds) 39 Influence of the potential-energy function on vibration-rotational wavefunctions and matrix elements of diatomic molecules Journal of Molecular Structure 35 (1976) 1-55 (with R. H. Tipping) 40 Potential-energy effects on cluster formation Faraday Discussions of the Chemical Society 61 (1976) 63-64 41 Perpendicular component of dipole moment in methyl groups Theoretica Chimica Acta 44 (1977) 215 42 Radial matrix elements and dipole-moment function of the ground state of CO Journal of Molecular Spectroscopy 65 (1977) 306-312 (with S. M. Kirschner, R. J. LeRoy and R. H. Tipping) 43 Dunham energy parameters of isotopic carbon oxide, hydrogen halide and hydroxyl radical molecules Journal of Molecular Spectroscopy 69 (1978) 169-172 44 Photochemical oxidation of iodosilane in solid argon Berichte der Bunsen Gesellschaft fur Physikalische Chemie 82 (1978) 105 (with V. R. Salares and M. J. Newlands) 45 Dipole-moment functions of the hydrogen halides Journal of Chemical Physics 73 (1980) 5221-5229 (with W. R. Rodwell and R. H. Tipping) 46 Statistical correlation of molecular structure with boiling points of N-heterocyclic compounds: multiple linear regression analysis Computers in Chemistry 5 (1981) 33-40 (with M. A. Abu-Elgheit) 47 Structures and dipole moments of nonionic nitrite rotamers Journal of Molecular Structure 75 (1981) 255-264 (with M. H. A. Hasan) 48 A general potential-energy function for diatomic molecules Proceedings of the Royal Society London A378 (1981) 287-300; A381 (1982) 479 49 Further Dunham energy coefficients of diatomic molecules Journal of Quantitative Spectroscopy and Radiative Transfer, 27 (1982) 481-482 (with J. P. Bouanich) 50 Precise potential-energy function for the state  ${}^{1}\Sigma^{+}$  of hydrogen chloride Journal of the Chemical Society Faraday Transactions II, 78 (1982) 1345-1362 (with J. A. Coxon) 51 Quantum-chemical computations on rotational isomers of hydrogen nitrite and nitritomethane Proceedings of the Royal Society London A381 (1982) 443-455 (with L. Farnell) 52 Applications of computer algebra in physical chemistry Computers in Chemistry 6 (1982) 169-172 53 Comparison of model potential-energy functions with their representations by a flexible polynomial Canadian Journal of Spectroscopy 27 (1982) 152-155 54 Herman-Wallis factors for higher overtone bands: application to HCl Journal of Molecular Spectroscopy **96** (1982) 442-450 (with R. H. Tipping)

- 55 Bounded matrix elements for the quartic-anharmonic oscillator *Physical Review* **A27** (1983) 95-100 (with R. H. Tipping)
- 56 Spectroscopic energy coefficients for vibration-rotational states of dinuclear molecules Computer Physics Communications **30** (1983) 101-105
- 57 One-photon spectroscopy of vibration-rotational states of diatomic molecules International Reviews of Physical Chemistry **3** (1983) 3-38 (with R. H. Tipping)
- 58 Calculation of the vibration-rotational spectrum of NH<sup>+</sup> Journal of Molecular Spectroscopy **101** (1983) 104-132 (with L. Farnell)
- 59 Expectation values for Morse oscillators
   Journal of Chemical Physics 79 (1983) 2537-2540 (with R. H. Tipping)
- 60 Herman-Wallis factors for Raman transitions of <sup>1</sup>Σ-state diatomic molecules Journal of Raman Spectroscopy **15** (1984) 38-40 (with R. H. Tipping)
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- 62 Theoretical Herman-Wallis coefficients C<sup>7</sup><sub>0</sub> and D<sup>7</sup><sub>0</sub> and the dipole-moment function of HCl Journal of Quantitative Spectroscopy and Radiative Transfer, **33** (1985) 145-154 (with R. H. Tipping)
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- 68 Comment on "*Ab initio* calculations of doublet states of NH<sup>+</sup>" *Chemical Physics Letters* **137** (1987) 191-192 (with L. Farnell)
- 69 The analytic solution by computer algebra of some problems in the vibration-rotational spectroscopy of diatomic molecules

*Journal of Symbolic Computation* **3** (1987) 277-281; *SIGSAM Bull.* **21**, No. 1 (1987) 40 (with R. H. Tipping)

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- 73 An analytic representation of the radial dependence of adiabatic and nonadiabatic corrections from molecular spectra of diatomic molecules *Chemical Physics Letters* **140** (1987) 506-511
- 74 The direct computation of the intensity of amplified lines
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- 75 Extension of a general potential-energy function for diatomic molecules Journal of Chemical Physics 88 (1988) 2804-2808
- 76 The analytic representation of radial functions determined from spectra of diatomic molecules Journal of Molecular Spectroscopy **128** (1988) 216-220

- 77 Line strengths of the band  $a {}^{1}\Delta_{g} v'=0 X {}^{3}\Sigma_{g} {}^{-} v''=0$  of  ${}^{16}O_{2}$ *Journal of Quantitative Spectroscopy and Radiative Transfer*, **39** (1988) 375-380 (with Y. P. Lee and L. B. Lin)
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- 79 The radial dependence of nonmechanical properties of diatomic molecules *Canadian Journal of Spectroscopy* **33** (1988) 72-74
- 80 Strengths of absorption lines in the vibration-rotational band v=5 v=0 of NO X  $^{2}\Pi_{r}$ Infrared Physics **28** (1988) 321-324 (with Y. P. Lee)
- 81 Radial functions from the hyperfine spectrum of NaBr Journal of Molecular Spectroscopy **131** (1988) 340-342
- 82 The infrared absorption spectrum of hydroxyl radicals in solid argon Chemical Physics Letters **151** (1988) 109-115 (with B. M. Cheng and Y. P. Lee)
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- 84 The inversion of spectral data for spin-orbital interaction in the hydroxyl radical, OH  $X^2$ Π. *Physica Scripta*, **38** (1988) 802-805
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- 87 Comment on "*Ab initio* molecular orbital calculation of the methyl nitrite syn-anti isomerization potential"

Chemical Physics Letters 156 (1989) 129-130 (with L. Farnell)

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- 93 Mesophases I Journal of the Chinese Chemical Society **36** (1989) 375-388
- 94 Mesophases II
  - Journal of the Chinese Chemical Society 36 (1989) 501-513
- 95 Determination of radial functions from vibration-rotational energies of the ground electronic state  $X^{1}\Sigma^{+}$  of hydrogen fluoride

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- 97 Comment on "Further contributions to the energy levels of a perturbed anharmonic oscillator -- application to adiabatic corrections"
  - Journal of Chemical Physics 92 (1990) 816
- 98 The nature of the chemical bond–1990 Journal of Chemical Education **67** (1990) 280-289
- 99 The diatomic rotating vibrator according to classical mechanics *Chinese Journal of Physics* **28** (1990) 237-251 (with R. H. Tipping)
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- 103 Application of spreadsheet programs for analysis of vibration-rotational bands Spectroscopy Letters 24 (1991) 345-350 (with F. Y. H. Wang)
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- 105 Radial functions of the molecule CH in electronic state  $X^{2}\Pi$ *Chinese Journal of Physics* **29** (1991) 213-221 (with F. Y. H. Wang)
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- 107 The vibration-rotational bands v<sub>3</sub>, 2v<sub>3</sub>-v<sub>3</sub> and v<sub>3</sub>+v<sub>6</sub>-v<sub>6</sub> of H<sub>3</sub>CF Journal of Molecular Spectroscopy 149 (1991) 109-124 (with D. Papousek, S. Civis and M. Winnewisser)
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- 109 Radial functions of SiS  $X^{1}\Sigma^{+}$  from vibration-rotational spectra Chemical Physics Letters **183** (1991) 40-44
- 110 Does He<sub>2</sub> exist? Journal of the Chinese Chemical Society **38** (1991) 425-427 (with F. Y. H. Wang)
- 111 Radial functions and the nature of the binding in LiCl and LiBr Journal of Molecular Structure 263 (1991) 167-175 (with M. C. C. Ho)
- 112 An analytic treatment of adiabatic and nonadiabatic effects on vibration-rotational energies of diatomic molecules

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- 114 Application of perturbation theory to vibration-rotational energies of diatomic molecules Journal of Physics **B25** (1992) 1375-1384 (with F. M. Fernandez)
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- 117 Vibration-rotational Einstein coefficients for HF/DF and HCl/DCl
   Journal of Chemical Physics 97 (1992) 1734-1741 (with E. Arunan and D. W. Setser)
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- Journal of the Chinese Chemical Society 39 (1992) 381-385
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- 121 Radial functions of the molecular cation  $ArH^+ X \Sigma^+$  from vibration-rotational spectra Journal of Molecular Spectroscopy **156** (1992) 8-14
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- 171 Teaching and doing mathematics with symbolic computation *Proceedings of the Eighth Asian Technology Conference Mathematics* (2003), **1**, 16 – 22
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