Quantum Mechanics of the Diatomic Molecule (Second Edition)

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IOP Series in Coherent Sources, Quantum Fundamentals, and Applications

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F J Duarte is a laser physicist based in Western New York, USA. His career has covered three continents while contributing within the academic, industrial, and defense sectors. Duarte is editor/author of 15 laser optics books and sole author of three books: *Tunable Laser Optics, Quantum Optics for Engineers*, and *Fundamentals of Quantum Entanglement*. Duarte has made original contributions in the fields of coherent imaging, directed energy, high-power tunable lasers, laser metrology, liquid and solid-state organic gain media, narrow-linewidth tunable laser oscillators, organic semiconductor coherent emission, *N*-slit quantum interferometry, polarization rotation, quantum entanglement, and space-to-space secure interferometric communications. He is also the author of the generalized multiple-prism grating dispersion theory and pioneered the use of Dirac's quantum notation in *N*-slit interferometry and classical optics. His contributions have found applications in numerous fields, including astronomical instrumentation, dispersive optics, femtosecond laser microscopy, geodesics, gravitational lensing, heat transfer, laser isotope separation, laser medicine, laser pulse compression, laser spectroscopy, mathematical transforms, nonlinear optics, polarization optics, and tunable diode-laser design. Duarte was elected Fellow of the Australian Institute of Physics in 1987 and Fellow of the Optical Society of America in 1993. He has received various recognitions, including the *Paul F Foreman Engineering Excellence Award* and the *David Richardson Medal* from the Optical Society.

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To John, Anna, and Melissa

To Justin, Jason, and Jola

Contents

Preface

0.1 First edition

The book notes from J O Hornkohl and extensive scientific discussions and research engagements in my work at the University of Tennessee Space Institute, Center for Laser Applications, motivate completion of this ebook. Communication exchanges occurred since the spring of 1987, and continued regularly until winter 2017 [1]. Over the years, several colleagues and postgraduate MSc and PhD students have contributed to applications of fundamental insights in the physics of the diatomic molecule. Thanks go to David Plemmons, Guoming Guan, Ying-Ling Chen, Wenhong Qin, Ivan Dors, Alexander Woods, David Surmick, Michael Witte, Ghaneshwar Gautam, and Christopher Helstern.

Significant emphasis has been placed on the application of the diatomic spectroscopy predictions in analysis of experimental data. For this reason, this ebook includes several chapters on applications in studies of diatomic molecules, especially important molecules such as cyanide (CN), aluminum monoxide (AlO), diatomic carbon (C_2), titanium monoxide (TiO), hydroxyl (OH), but also selected work on other diatomic molecules.

This text introduces insights that are essential in utilizing the inherent symmetries associated with diatomic molecules. Consequently, line positions and strengths associated with transitions from lower and upper state-manifolds are determined without invoking approximations that separate vibrations and rotations of diatomic nuclei from electron motion based on mass. The approach utilized in this work makes use of the separation of angular coordinates from electronic vibrational coordinates. Consequently, the volley of selection rules for diatomic spectroscopy is no longer required, including methodologies that rely on so-called reversed angular momentum techniques.

This work summarizes well over 30 years of quantitative analysis of temporally and spatially resolved experimental records, almost all of the experiments discussed in this ebook were conducted at the Center for Laser Applications (CLA) at the University of Tennessee Space Institute. Applications include understanding on nonequilibrium fluid and plasma physics and interpretation of stellar astrophysics spectra. In several cases of laser-induced plasma investigations, both atomic and molecular signatures or superposed spectral characteristics from molecules and atoms can be identified. Analysis of such superposition spectra requires accurate knowledge of wavelength positions and transition strengths. The revival and replacement of electrical-spark spectroscopy with laser-spark or laser-plasma spectroscopy for quantitative elemental composition analysis since the mid-1990s, viz. laser-induced breakdown spectroscopy (LIBS), extends into increased interests in molecular LIBS since (give-or-take) the mid-2000s. From an analytical and practical point of view, the requirements can be reduced to the availability of a set of diatomic line-strengths in tabular form along with programs that are designed to appropriately read the records. However, this ebook provides a reasonable account of the quantum mechanics of the diatomic molecule, along with selected applications that were important for motivating a consistent approach and for analyzing recorded data sets from various experiments in the CLA laboratories.

The challenge of this work has been the prediction of spectra with a focus on diatomic spectroscopy. The aim of the lifetime work of Jim Hornkohl is the design of an algorithm to predict and fit computed and measured molecular spectra to provide inferences on parameters such as excitation temperature. The means to accomplish goals for various diatomic molecules are the consistent application of standard quantum theory of angular momentum. During his career, Jim engaged in efforts to overcome techniques such as Van Vleck's reversed angular momentum approach based on angular momentum commutators. The apparent difficulties included the battles with the established practice to predict and compute spectra and design programs despite the mathematical inconsistencies associated with the reversed angular momentum practice. The experimental investigations, and again the stimulating discussions, motivated refinements such as enlarging the data sets for the CN, C_2, or TiO diatomic molecules. In turn, the discussed applications in this book are intended to alleviate analysis of diatomic spectra composed of superpositions of a significant amount of transition lines within typical resolution for laser-plasma emission spectroscopy, to name but one example.

Christian Parigger
August 2019

0.2 Second edition

The second edition includes 10 additional chapters, one on the fundamentals and nine on the applications parts. Three additional appendices are included, namely: communication of NMT and BESP scripts for computation of diatomic spectra, Abel inversion scripts with one specific example, and an appendix on select recent publications that include C.G.P. as author. The additions primarily address communication of spatial profiles analyses, including Abel inversion and communication of scripts for diatomic spectroscopy and Abel inversions. However, comparisons with other existing databases clearly reveal the significance of the line strengths for the selected electronic transitions of diatomic molecules. The comparisons also include a section of C_2 laser-induced fluorescence. The existing databases comparisons include PGOPHER, LIFBASE, and ExoMol databases that are compared with line-strength data of diatomic molecules of interest, particularly for laser-induced plasma that is generated in gases and gas mixtures.

- New chapter 2 addresses the foundations of quantum mechanics and the mathematical implementation of specific symmetries. Application of the correspondence principle, relating classical and quantum mechanics, leads to the occurrence of the infamous sign-reversal. This chapter addresses formal treatment of symmetries in quantum mechanics. Quantum theory contraindicates sign changes of the fundamental angular momentum algebra.

Reversed angular momentum sign changes are of a heuristic nature and are actually undesirable in the analysis of diatomic spectra.

- New chapter 15 communicates line-strength data and associated scripts for the computation and spectroscopic fitting of selected transitions of diatomic molecules. The scripts for data analysis are designed for inclusion in various software packages or program languages. Selected results demonstrate the applicability of the program for data analysis in laser-induced optical breakdown spectroscopy, primarily at the University of Tennessee Space Institute, Center for Laser Applications. Representative spectra are calculated and referenced to measured data records. Comparisons of experiment data with predictions from other tabulated diatomic molecular databases confirm the accuracy of the communicated line-strength data.
- New chapter 17 discusses cavity ring-down spectroscopy of methylidyne in a chemiluminescent plasma that is produced in a microwave cavity. Of interest are the rotational lines of selected vibrational transitions for the A–X and B–X bands. This chapter also includes recent analysis that shows excellent agreement of measured and computed data, and it communicates CH line-strength data. The CH radical is an important diatomic molecule in hydrocarbon combustion diagnosis and analysis of stellar plasma emissions, to name just two examples for analytical plasma chemistry.
- New chapter 19 discusses diatomic molecular spectroscopy of laser-induced plasma and analysis of data records, specifically signatures of cyanide (CN). Line-strength data from various databases are compared for simulation of the cyanide spectra. Of interest are recent predictions using an astrophysical database, i.e., ExoMol, a laser-induced fluorescence database, i.e., LIFBASE, and a program for simulating rotational, vibrational, and electronic spectra, i.e., PGOPHER.
- New chapter 21 presents analysis of carbon Swan bands laser-plasma emission records using line-strength data and the ExoMol database. The temperature inferences are elaborated when using nonlinear fitting with both databases. The line-strength data are also utilized for analysis of laser-induced fluorescence experiments that employ a spectral resolution of the order of 5 pm. Accurate diatomic carbon databases show many applications in laboratory diagnosis and interpretation of astrophysical plasma records.
- New chapter 23 elaborates on analysis of aluminum monoxide (AlO), laser-plasma emission records using line-strength data, and the ExoMol astrophysical database. A nonlinear fitting program computes comparisons of measured and simulated diatomic molecular spectra. This work also presents a comparison of the AlO line strength and of ExoMol data for the AlO diatomic molecule. Accurate AlO databases show a volley of applications in laboratory and astrophysical plasma diagnosis.
- New chapter 25 applies NMT and BESP scripts for the fitting of recorded experimental hydroxyl data. The fitting program also incorporates a slight, overall wavelength offset. The ExoMol and line-strength data yield close to identical temperature with a slightly different linear background.

The databases for specific hydroxyl transition yield similar predictions of the recorded laser-plasma spectra for time delays of the order of one hundred microseconds after optical breakdown initiation.

- New chapter 26 communicates measurement and analysis of diatomic molecular hydroxyl spectra after generation of laser-induced plasma, and it also shows details of the expanding plasma including associations of shadowgraphs with spectroscopy. Formation of OH is clearly discernible at time delays of several dozen microseconds after plasma initiation. Optical emissions are dispersed by a Czerny–Turner spectrometer and an intensified charge-coupled device records the data along the wavelength and slit dimensions.
- New chapter 29 combines time-resolved emission spectroscopy with Abel integral inversion techniques to obtain radial electron density values in laser-induced plasma. This chapter also includes details of the Abel transforms Hydrogen beta line profiles are recorded following optical breakdown in ultra-high-pure hydrogen gas. Asymmetric Abel inversion techniques are utilized in the analysis of collected, time-resolved data. The averaged, line-of-sight electron densities are found to be in of the order of one hundredth of an amagat for time delays close to one-half microseconds. The electron densities indicate variations across the laser-induced plasma.
- New chapter 30 elucidates the connection of measured shadowgraphs from optically induced air breakdown with emission spectroscopy in selected gas mixtures. Spectroscopic analysis explores well-above hypersonic expansion dynamics using primarily diatomic molecule cyanide and atomic hydrogen emission spectroscopy. Analysis of the air breakdown and selected gas breakdown events permits the use of Abel inversion for inference of the expanding species distribution. Typically, species are prevalent at higher density near the hypersonically expanding shock wave, measured by tracing cyanide and a specific carbon atomic line.
- New appendix J presents NMT and BESP MATLAB-scripts for computation of diatomic spectra.
- New appendix K presents Abel inversion MATLAB-scripts with one specific example.
- New appendix L summarizes select recent publications that include C.G.P. as author.

Christian Parigger
February 2024

Reference

[1] Parigger C G and Nemes L 2017 *Int. J. Mol. Theor. Phys.* **1** 00105

Acknowledgements

CGP and JOH appreciate the support by the Center for Laser Applications (CLA) at the University of Tennessee Space Institute during over 30 years of research engagement in spectroscopy. The research led to this book and its second edition that describe how quantum mechanics can be used to predict diatomic molecule spectra. The book and its second edition provide a comprehensive overview on diatomic molecule fundamentals and emphasize the applications of spectroscopy predictions in analysis of experimental data. Both CGP and JOH are happy to report interests and contributions by postgraduate students. Moreover, CGP is delighted about publication of the first and second editions in memoriam to JOH, a long time collaborator in analysis of laser-induced plasma spectra recorded at the CLA. Last but not least, CGP thanks researchers and colleagues at the CLA and international collaborators throughout the world for extensive discussions and motivation towards completion of both book editions.

Author biographies

Christian G. Parigger

Christian G. Parigger (Courtesy UTSI photo albums: L Horton.)

The research interests of Dr Christian Parigger include fundamental and applied spectroscopy, nonlinear optics, quantum optics, ultrafast phenomena, ultrasensitive diagnostics, lasers, combustion and plasma physics, optical diagnostics, biomedical applications, and, in general, atomic and molecular and optical physics. His Mag. rer. nat. degree shows work on optical bistability at the University of Innsbruck, Austria, with guidance by Dr Peter Zoller. His PhD degree studies are on the subject of polarization spectroscopy and magnetically induced switching at the University of Otago, Dunedin, New Zealand, with guidance by Drs Wes Sandle and Rob Ballagh. He also holds the Dr rer. nat. degree in Physics from the University of Innsbruck, Austria. Since 1987, his work encompasses experimental, theoretical and computational research, together with teaching, service, and outreach at the Center for Laser Applications at The University of Tennessee Space Institute, Tullahoma, Tennessee, USA.

James O and Jeri Hornkohl

James O and Jeri Hornkohl (Courtesy UTSI photo albums: L Horton.)

The contributions of James Hornkohl, or 'Jim', encompass the spectroscopy of diatomic molecules, and the application of such spectroscopy in diagnosis of combustion, plasmas, rocket propulsion, and related problems. His support of student theses and dissertations has been especially significant, including the application of numerical methods in analysis of experiments. Moreover, his help has been greatly appreciated by his collaborators in the design of computational and experimental methods to record digital data. During the last 30 years prior to his death on February 7, 2017, Jim had been strongly engaged in the description of the very details on diatomic spectroscopy. The challenge to Jim's work has been the prediction of spectra with a focus on diatomic spectroscopy. The aim of his lifetime work was the design of an algorithm for the prediction and fitting of computed to measured molecular spectra and to provide inferences of parameters such as excitation temperature. The means to accomplish goals for various transitions of diatomic molecules are the consistent application of standard quantum theory of angular momentum.

Part I

Fundamentals of the diatomic molecule

Christian G Parigger and James O Hornkohl

Chapter 1

Primer on diatomic spectroscopy

1.1 Overview

This book describes how one uses quantum mechanics to predict the spectra of diatomic molecules in their gaseous state. The two most important attributes of a spectral line are its position in the electromagnetic spectrum and the strength with which the molecule can interact with the radiation field to produce spectral lines. Thus, a book that discusses the calculation of positions and intensities of spectral lines of a diatomic molecule equally communicates the application of quantum theory to the diatomic molecule.

The theoretically convenient measure of spectral line position is its vacuum wave number $\tilde{\nu}_{u\ell}$, which is the difference between the upper term T_u (i.e., upper energy eigenvalue expressed in the units of cm^{-1}) and the lower term T_ℓ,

$$\tilde{\nu}_{u\ell} = T_u - T_\ell. \tag{1.1}$$

In the optical region, the term difference corresponds to a specific color. However, experiments usually measure the wavelength positions in a laboratory setting at standard ambient temperature and pressure. For typical laser spectroscopy investigations of, say, optical emission spectroscopy subsequent to generation of a laser spark, spectral resolutions of the instrument spectrometer and detector amount to 0.1–0.01 nm, rarely to 0.001 nm or 1 pm. At the wavelength, λ, of 400 nm, a spectral resolution, $\Delta\lambda$, of better than 1 pm corresponds to a resolving power, R,

$$R = \lambda/\Delta\lambda \geqslant 400\,000, \tag{1.2}$$

or a wave number resolution of better than 0.05 cm^{-1}. The spectral resolution of diatomic molecular data computed in this book is better than 0.05 cm^{-1}. For laser-induced optical breakdown experiments, which is a recent application of diatomic molecular spectroscopy, resolving powers are of the order of 4000–10 000. For high-resolution, absorption measurements of stellar astrophysical objects, resolving powers of the order of 40 000 are quite common.

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The theoretically most convenient measure of a molecule's ability to interact with electromagnetic radiation is its Condon and Shortley [1] line strength, $S_{u\ell}$, which describes transitions between an upper, u, and a lower level, ℓ. The line strength represents a summation over individual states that comprise upper and lower levels. Both the vacuum wave number $\tilde{\nu}_{u\ell} = \tilde{\nu}_{\ell u}$ and the line strength $S_{u\ell} = S_{\ell u}$ are symmetric with regard to the upper and lower levels. In addition, the symbols u and ℓ represent a collection of quantum numbers. In diatomic spectroscopy, upper state quantum numbers are normally denoted with a single prime, while lower states are denoted with the absence of a prime or a double prime. The absence of a double prime has become the standard way of denoting a lower state diatomic quantum number.

1.2 Reversed angular momentum

Historically, the reversed-angular-momentum (RAM) methodology has successfully predicted diatomic spectra without the use of modern digital computers. The RAM method establishes a reduced set of basis states; in other words, works with an a priori approximation. Sets of rules are introduced when applying a transformation to a molecular-fixed from the laboratory-fixed coordinate system. These rules utilize a supposed reversal of sign in the application of quantum mechanical angular momentum algebra. This section provides a brief historic account of the challenges associated with the RAM method.

The reversed-angular momentum approach is mentioned first in an article on the quantization question of the asymmetric top [2]. Klein writes in the introduction that the paper might be of interest for methods of quantization. The reversed sign is introduced for the equations of the components of angular momentum in the molecular-fixed coordinate system in order to obtain agreement with the well-established classical equations for the symmetric top. Conversely, the application of the standard, laboratory-fixed angular momentum equations would lead to the wrong classical result. This article also makes reference to canonical conjugate Euler angles that are interpreted as references to dual space.

The RAM methodology is embraced by Van Vleck in his work on the coupling of angular momentum vectors in molecules [3]. Notably, Sir Harold Kroto communicates in his acceptance lecture for the 1996 Nobel Prize in Chemistry, 'Symmetry, Space, Stars and C_{60}' [4], the importance of 'Symmetry, the Key to the Theory of Everything'. With reference to the RAM work, Sir Kroto quotes Van Vleck: '*Practically every-one (!) knows that the components of total angular momentum (NB the angular momentum operator is usually denoted by* J *and the associated quantum number by* j*) of the molecule relative to the axes [x, y, z] fixed in space satisfy the commutation relation of the form*

$$J_x J_y - J_y J_x = iJ_z \tag{1.3}$$

Klein discovered the rather surprising fact that when total angular momentum is referred to axes mounted in the molecule which we will denote by [x', y', z'] the sign of i in the commutation relation is reversed i.e.

$$J_{x'}J_{y'} - J_{y'}J_{x'} = -iJ_{z'} \tag{1.4}$$

Sir Kroto goes on to say: *Does practically everyone know this?—I wondered whether to check this claim out by asking everyone on the main street in Brighton whether they did. I hardly knew—or more accurately—really understood the first relation, let alone the second. However I did know that angular momentum was quantised and governed by the fundamental relations*

$$\langle j|J^2|\rangle = \hbar j(j+1) \tag{1.5}$$

$$M_J = -j \ldots +j \tag{1.6}$$

which means that J has $2j + 1$ *possible orientations, and*

$$\Delta j = 0, \pm 1 \tag{1.7}$$

which indicates that when a transition occurs, j may only change by one unit or on occasion remain unchanged.' Previously, in 1975 and then in 1992, Sir Kroto discussed the molecule-fixed angular momentum following Van Vleck [3], leading to the reversed-angular momentum equations in his Nobel laureate lecture [4] and in his book on molecular rotation spectra [5].

However, an accurate review shows that there is no reversal of the sign when moving from a laboratory-fixed to a molecule-fixed coordinate system; in other words, there is no mathematical support of the reversed sign. Sustenance of the angular momentum equations can be explained as follows. In terms of classical mechanics, reversal of motion occurs as one goes from a rotating system to a fixed system, or vice versa. For example, motion reversal can be experienced by looking at the surroundings while on a rotating merry-go-round versus observing the rotation in the fixed reference frame. The quantum mechanical implementation of motion reversal or time reversal changes the sign and takes the conjugate complex, leading to the preservation of the sign. Reference to dual space would confuse things because clearly the standard angular momentum operator equations are not affected by a transformation from laboratory-fixed to molecule-fixed coordinates (see appendix A).

A reasonably concise treatment shows preservation of the commutator relations under a unitary transformation. Consider the operators A, B, and C which satisfy the commutation formula

$$AB - BA = iC \tag{1.8}$$

and subject these three operators to the unitary transformation U; that is,

$$A' = U^\dagger\, A\, U \tag{1.9a}$$

$$A = U\, A'\, U^\dagger \tag{1.9b}$$

with similar equations holding for B and C. Then,

$$AB - BA = U\, A'\, U^\dagger\, U\, B'\, U^\dagger - U\, B'\, U^\dagger\, U\, A'\, U^\dagger \tag{1.10a}$$

$$= U\ A'\ B'\ U^{\dagger} \tag{1.10b}$$

$$= iC \tag{1.10c}$$

$$iU^{\dagger}\ C\ U = A'B' \tag{1.10d}$$

$$iC' = A'B' - B'A'. \tag{1.10e}$$

The above result, e.g., see Davydov [6], holds for all commutators, including those for angular momentum. Thus,

$$J_{x'}J_{y'} - J_{y'}J_{x'} = i\ J_{z'} \tag{1.11a}$$

$$J_{y'}J_{z'} - J_{z'}J_{y'} = i\ J_{x'} \tag{1.11b}$$

$$J_{z'}J_{x'} - J_{x'}J_{z'} = i\ J_{y'} \tag{1.11c}$$

In summary, the RAM method is not utilized in this book for the computation of diatomic molecular spectra. RAM is avoided due, in part, to not needing approximations thanks to the availability of modern digital computers and due in part to the mathematical inconsistency of the supposed change of sign, as implied by the 'reversed-angular momentum' descriptive nomenclature.

1.3 Exact diatomic eigenfunction

An exact expression of the diatomic eigenfunction is essential for prediction of spectra. The major difference between this book and other treatments of the diatomic molecule is the use of the Wigner–Witmer diatomic eigenfunction [7] in place of invoking the Born–Oppenheimer approximation [8] from the very beginning of a theory description. In the Wigner–Witmer approach, angular coordinates are exactly separated from the electronic–vibrational coordinates. In this book, the Wigner–Witmer eigenfunction is employed for computation of the vacuum wave numbers and the rotational line strengths. If one were to instead adopt the Born–Oppenheimer approximation, then the rotational line strengths would be labeled as Hönl–London factors. The Born–Oppenheimer approximation breaks the electronic–vibrational strength into electronic and vibrational parts that correspond to *r*-centroids and Franck–Condon factors, and both may be functions of the total angular momentum in the upper and lower levels.

The expression *spectroscopic accuracy* refers to the accuracy with which line position measurements can be performed. Whereas wavelength measurements having an accuracy of 1 part per million are routinely performed, achieving an accuracy of 1 part per hundred in the measurement of relative intensities of a group of spectral lines is fully adequate for many purposes. Thus, one may elect to directly use the Born–Oppenheimer approximation for many practical calculations of molecular line intensity; namely, approximating the diatomic eigenfunction as a product of electronic, vibrational, and rotational factors. However, the Born–Oppenheimer approximation cannot produce diatomic term values with spectroscopic accuracy without generalization. To achieve spectroscopic accuracy within the Born–Oppenheimer approximation, one must include sums over the many electronic states of the molecule and sums over the many vibrational states of each electronic state. Van Vleck transformations [9] or other mathematical procedures reduce the dimension of the Hamiltonian matrix prior to numerically diagonalization [10–15].

In this book, only one diatomic selection rule is used. A spectral line, i.e., a term difference, is allowed if the angular momentum part of its line strength is non-vanishing. However, a modification of the line strength computation is required if the diatomic molecule in question is homonuclear, i.e., the two nuclei are identical. An unresolved hyperfine structure in the spectrum of a homonuclear molecule causes states of positive parity and negative parity to have different nuclear spin statistical weights, g_+ and g_-. If the nuclear spin is zero, then either g_+ or g_- will be zero. Thus, exchange symmetry, the symmetry associated with the exchange of identical particles, rigorously forbids certain spectral lines, even when the rotational line strength is nonzero. However, if the rotational line strength factor vanishes, then the spectral line is rigorously forbidden.

1.4 Computation of diatomic spectra

The required steps for computation of spectra can be summarized as follows:

- An angular momentum momentum coupling model must be chosen because angular momentum theory does not tell us how the total angular momentum is formed from the orbital and spin momenta.
- The eigenfunctions for everything in the system except the total angular momentum are computed.
- With the eigenfunctions obtained in the previous step and the chosen angular momentum coupling model, upper and lower Hamiltonians are computed and diagonalized.
- From the orthogonal matrices that diagonalize the upper and lower Hamiltonians, the line strengths are computed for various possible types of transitions, e.g., electric dipole, magnetic dipole, electric quadrupole, etc. Typically, one knows precisely what type of transition dominates in the spectrum, but this is not invariably the case.
- The nonvanishing of the rotational angular momentum part of the line strength selects the subset of allowed spectral lines from the computed term differences.

Consequently, the minimal information required for computation of a spectrum includes selected term differences $\tilde{\nu}_{u\ell}$ and the computed line strengths $S_{u\ell}$. A description of a diatomic molecule having N electrons and residing in field free space requires $3N + 6$ spatial or angular coordinates, the time t, N electronic spin variables, and two nuclear spin variables. In the case of the diatomic molecule, the only exactly separable variables are the time t, the coordinates of the total mass, and three Euler angles which describe the total angular momentum. The Wigner–Witmer diatomic eigenfunction provides the exact separation of three Euler angles, but $3N$ internal spatial coordinates and the numerous spins remain. Unless the number of electrons N is very small, the diatomic problem remains unsolvable with spectroscopic accuracy because there are $3N$ independent variables that cannot be treated with mathematical exactness.

Despite the challenges mentioned in the previous paragraph, one can, with two stringent caveats, apply the above algorithm to the diatomic molecule. The first caveat is that one must have extensive experimentally recorded wave number tables, $\tilde{\nu}_{u\ell}^{\mathrm{exp}}(J', J)$, versus upper and lower total angular momenta, J' and J, respectively, for many vibrational bands in the spectrum of a molecule of interest. The second caveat is associated with using trial values of semiempirical molecular parameters for each vibrational level, v, such as B_v, D_v, A_v, λ_v, γ_v, and so on. One computes term differences, $\tilde{\nu}_{u\ell}(J', J)$, from numerically diagonalized upper and lower Hamiltonians, calculates corrections to the trial values of the parameters from differences $\tilde{\nu}_{u\ell}(J', J) - \tilde{\nu}_{u\ell}^{\mathrm{exp}}(J', J)$, and iterates the computations until the errors in the computed line positions are comparable to the estimated errors in the experimental line positions. When successful, this procedure yields working models for the upper and lower Hamiltonians and sets of molecular parameters that predict the measured line positions.

The practical significance of molecular parameters was their appearance in term value equations, semiempirical equations with which one can compute the upper T_u and lower T_ℓ terms, and thereby the vacuum wave number $\tilde{\nu}_{u\ell}$. Herzberg [16] gives many examples of term value equations, but note that when Herzberg wrote his book the numerical diagonalization of thousands of matrices was impractical. The current significance of the molecular parameters is that they can be used to compute diatomic Hamiltonian matrix representations in one of the Hund's bases.

In this book the computation of $\tilde{\nu}_{u\ell}(J', J)$ and $S_{u\ell}(J', J)$ is based upon the Wigner–Witmer diatomic eigenfunction instead of the eigenfunction associated with the Born–Oppenheimer approximation, but computations of the electronic–vibrational strengths utilize separation of electronic from vibrational contributions familiar from the Born–Oppenheimer approximation.

References

[1] Condon E U and Shortley G 1953 *The Theory of Atomic Spectra* (Cambridge: Cambridge University Press)

[2] Klein O 1929 Zur Frage der Quantelung des asymmetrischen Kreisels *Z. Phys.* **58** 730

[3] Van Vleck J H 1951 The coupling of angular momentum vectors in molecules *Rev. Mod. Phys.* **23** 213

[4] Kroto H W 1996 Symmetry, space, stars and C_{60}, 1996 (accessed 19 January 2016). https://www.nobelprize.org/prizes/chemistry/1996/kroto/facts/

[5] Kroto H W 1992 *Molecular Rotation Spectra* (New York: Dover)

[6] Davydov A S 1965 *Quantum Mechanics* (Oxford: Pergamon)

[7] Wigner E and Witmer E E 1928 *Z. Phys.* **51** 859
Hettema H 2000 *Quantum Chemistry: Classic Scientific Papers* p 287 (Singapore: World Scientific)

[8] Born M and Oppenheimer R 1927 *Ann. Phys.* **84** 457
Hettema H 2000 *Quantum Chemistry: Classic Scientific Papers* p 1 (Singapore: World Scientific)
[9] Kemble E C 2005 *The Fundamental Principles of Quantum Mechanics* (Mineola, NY: Dover)
[10] Zare R N, Schmeltekopf A L, Harrop W J and Albritton D L 1973 *J. Mol. Spectrosc.* **46** 37
[11] Bunker P R and Jensen P 1998 *Molecular Symmetry and Spectroscopy* 2nd edn (Ottawa: NRC)
[12] Brown J M and Carrington A 2003 *Rotational Spectroscopy of Diatomic Molecules* (Cambridge: Cambridge University Press)
[13] Lefebvre-Brion H and Field R W 2004 *The Spectra and Dynamics of Diatomic Molecules* (New York: Elsevier/Academic)
[14] James K G 2005 Watson. Different forms of effective hamiltonians *J. Mol. Spectrosc.* **103** 3283
[15] Field R W, Baraban J H, Lipoff S H and Annelise R B 2011 Effective hamiltonians for electronic fine structure and polyatomic molecules *Handbook of High-Resolution Spectroscopy* ed M Quack and F Merkt (New York: Wiley)
[16] Herzberg G 1950 Molecular Spectra and Molecular Structure I *Spectra of Diatomic Molecules* 2nd edn (New York: Van Nostrand Reinhold)

Full list of references

Prelims

[1] Parigger C G and Nemes L 2017 *Int. J. Mol. Theor. Phys.* **1** 00105

Chapter 1

[1] Condon E U and Shortley G 1953 *The Theory of Atomic Spectra* (Cambridge: Cambridge University Press)
[2] Klein O 1929 Zur Frage der Quantelung des asymmetrischen Kreisels *Z. Phys.* **58** 730
[3] Van Vleck J H 1951 The coupling of angular momentum vectors in molecules *Rev. Mod. Phys.* **23** 213
[4] Kroto H W 1996 Symmetry, space, stars and C_{60}, 1996 (accessed 19 January 2016). https://www.nobelprize.org/prizes/chemistry/1996/kroto/facts/
[5] Kroto H W 1992 *Molecular Rotation Spectra* (New York: Dover)
[6] Davydov A S 1965 *Quantum Mechanics* (Oxford: Pergamon)
[7] Wigner E and Witmer E E 1928 *Z. Phys.* **51** 859
Hettema H 2000 *Quantum Chemistry: Classic Scientific Papers* p 287 (Singapore: World Scientific)
[8] Born M and Oppenheimer R 1927 *Ann. Phys.* **84** 457
Hettema H 2000 *Quantum Chemistry: Classic Scientific Papers* p 1 (Singapore: World Scientific)
[9] Kemble E C 2005 *The Fundamental Principles of Quantum Mechanics* (Mineola, NY: Dover)
[10] Zare R N, Schmeltekopf A L, Harrop W J and Albritton D L 1973 *J. Mol. Spectrosc.* **46** 37
[11] Bunker P R and Jensen P 1998 *Molecular Symmetry and Spectroscopy* 2nd edn (Ottawa: NRC)
[12] Brown J M and Carrington A 2003 *Rotational Spectroscopy of Diatomic Molecules* (Cambridge: Cambridge University Press)
[13] Lefebvre-Brion H and Field R W 2004 *The Spectra and Dynamics of Diatomic Molecules* (New York: Elsevier/Academic)
[14] James K G 2005 Watson. Different forms of effective hamiltonians *J. Mol. Spectrosc.* **103** 3283
[15] Field R W, Baraban J H, Lipoff S H and Annelise R B 2011 Effective hamiltonians for electronic fine structure and polyatomic molecules *Handbook of High-Resolution Spectroscopy* ed M Quack and F Merkt (New York: Wiley)
[16] Herzberg G 1950 Molecular Spectra and Molecular Structure I *Spectra of Diatomic Molecules* 2nd edn (New York: Van Nostrand Reinhold)

Chapter 2

[1] Parigger C G 2021 *Foundations* **1** 208
[2] Klein O 1929 *Z. Phys.* **58** 730
[3] Van Vleck J H 1951 *Rev. Mod. Phys.* **23** 213
[4] Nöther E, Nachr , König D, Gesellsch and Wiss D 1918 *Nachr. D. König. Gesellsch. D. Wiss. Göttingen* **918** 235
[5] Nöther E 1971 *Transp. Theory Statist. Phys.* **1** 183
[6] Parigger C G 2021 *Foundations* **1** 208

[7] Condon E U and Shortley G 1953 *The Theory of Atomic Spectra* (Cambridge: Cambridge University Press)
[8] Parigger C G and Hornkohl J O 2020 *Quantum Mechanics of the Diatomic Molecule with Applications* (Bristol: IOP Publishing)
[9] Parigger C G and Hornkohl J O 2010 *Int. Rev. At. Mol. Phys.* **1** 25
[10] Dirac P A M 1926 *Proc. Roy. Soc. Lond. A* 111 281
[11] Heisenberg W, Born M and Jordan P 1926 *Z. Phys.* **35** 557
[12] Popper K 1992 The logic and evolution of scientific theory *All Life Is Problem Solving* (London: Routledge)
[13] Brown J and Carrington A 2003 *Rotational Spectroscopy of Diatomic Molecules* (Cambridge: Cambridge University Press)
[14] Lefebvre-Brion H and Field R W 2004 *The Spectra and Dynamics of Diatomic Molecules* (Amsterdam: Elsevier)
[15] Jensen P and Bunker P R 2005 *Fundamentals of Molecular Spectroscopy* (Bristol: IOP Publishing)
[16] Gottfried K 1989 *Quantum Mechanics* (Reading: Addison-Wesley)
[17] Baym G 1969 *Lectures on Quantum Mechanics* (Reading: Benjamin/Cummings)
[18] Shore B W and Menzel D H 1968 *Principles of Atomic Spectra* (Reading: Addison-Wesley)
[19] Judd B R 1975 *Angular Momentum Theory for Diatomic Molecules* (New York: Academic)
[20] Mizushima M 1975 *The theory of rotating diatomic molecules*
[21] Kovacs I 1969 *Rotational Structure in the Spectra of Diatomic Molecules* (New York: Elsevier)
[22] Hougen J T 1970 *The Calculation of Rotational Energy Levels and Rotational Line Intensities in Diatomic Molecules* volume NBS Monograph 115 (Washington, DC: U.S. Government Printing Office)
[23] Kroto H W 1992 *Molecular Rotation Spectra* (New York: Dover)
[24] Carrington A, Levy D H and Miller T A 1970 *Adv. Chem. Phys.* **18** 149
[25] Freed K F 1966 *J. Chem. Phys.* **45** 4214
[26] Cohen-Tannoudji C, Diu B and Laloe F 2019 *Quantum Mechanics, Volume 1: Basic Concepts, Tools, and Application* 2nd edn (Weinheim: Wiley-VCH)
[27] Cohen-Tannoudji C, Diu B and Laloe F 2019 *Quantum Mechanics, Volume 2: Angular Momentum, Spin, and Approximation Methods* 2nd edn (Weinheim: Wiley-VCH)
[28] Arfken G B, Weber H J and Harris F E 2012 *Mathematical Methods for Physicists, A Comprehensive Guide* 7th edn (New York: Academic)
[29] Western C M 2017 *J. Quant. Spectrosc. Radiat. Transf.* **186** 221
[30] Kunze H-J 2009 *Introduction to Plasma Spectroscopy* (Heidelberg: Springer)
[31] Demtröder W 2014 *Laser Spectroscopy 1: Basic Principles* 5th edn (Heidelberg: Springer)
[32] Demtröder W 2015 *Laser Spectroscopy 2: Experimental Techniques* 5th edn (Heidelberg: Springer)
[33] Hertel I V and Schulz C-P 2015 *Atoms, Molecules and Optical Physics 1, Atoms and Spectroscopy.* (Heidelberg: Springer)
[34] Hertel I V and Schulz C-P 2015 *Atoms, Molecules and Optical Physics 2, Molecules and Photons–Spectroscopy and Collisions* (Heidelberg: Springer)
[35] Radziemski L J and Cremers D E 2006 *Handbook of Laser-Induced Breakdown Spectroscopy* (New York: Wiley)

[36] Miziolek A W, Palleschi V and Schechter I 2006 *Laser Induced Breakdown Spectroscopy* (New York: Cambridge University Press)
[37] Singh J P and Thakur S N (ed) 2020 *Laser-Induced Breakdown Spectroscopy* 2nd edn (New York: Elsevier)
[38] Tennyson J, Lodi L, McKemmish L K and Yurchenko S N 2016 *aeXiv* p 1605.023 01v1
[39] Davydov A S 1965 *Quantum Mechanics* (Oxford: Pergamon)
[40] Wigmer E and Witmer E E 1928 *Z. Phys.* **51** 859
[41] Hettema E H 2000 *On the Structure of the Spectra of Two-Atomic Molecules According to Quantum Mechanics. In: Quantum Chemistry: Classic Scientific Papers* (Singapore: World Scientific)
[42] Bransden B H and Joachain C J 2003 *Physics of Atoms and Molecules* 2nd edn (Essex: Prentice-Hall)
[43] Parigger C G, Woods A C, Surmick D M, Gautam G, Witte M J and Hornkohl J O 2015 *Spectrochim. Acta* B **107** 132
[44] Parigger C G, Jordan H B S, Surmick D M and Splinter R 2020 *Molecules* **25** 988
[45] Parigger C G, Surmick D M, Helstern C M, Gautam G, Bol'shakov A A and Russo R 2020 *Molecular Laser-Induced Breakdown Spectroscopy. In: Laser Induced Breakdown Spectroscopy* ed J P Singh and S N Thakur 2nd edn (New York: Elsevier)
[46] Parigger C G, Helstern C M, Jordan B S, Surmick D M and Splinter R 2020 *Molecules* **25** 615

Chapter 3

[1] Condon E U and Shortley G 1953 *The Theory of Atomic Spectra* (Cambridge: Cambridge University Press)
[2] Wigner E and Witmer E E 1928 *Z. Phys.* **51** 859
Hettema H 2000 *Quantum Chemistry: Classic Scientific Papers* p 287 (Singapore: World Scientific)
[3] Born M and Oppenheimer R 1927 *Ann. Phys.* **84** 457
Hettema H 2000 *Quantum Chemistry: Classic Scientific Papers* p 1 (Singapore: World Scientific)

Chapter 4

[1] Arfken G B, Weber H J and Harris F E 2012 *Mathematical Methods for Physicists: A Comprehensive Guide* 7th edn (New York: Academic)
[2] Wolf A A 1969 *Am. J. Phys.* **37** 531
[3] Wigner E and Witmer E E 1928 *Z. Phys.* **51** 859
Hettema H 2000 *Quantum Chemistry: Classic Scientific Papers* p 287 (Singapore: World Scientific)

Chapter 5

[1] Wigner E and Witmer E E 1928 *Z. Phys.* **51** 859
Hettema H 2000 *Quantum Chemistry: Classic Scientific Papers* p 287 (Singapore: World Scientific)
[2] Weissbluth M 1978 *Atoms and Molecules* (New York: Academic)

Chapter 6

[1] Wigner E and Witmer E E 1928 *Z. Phys.* **51** 859 H. Hettema, *Quantum Chemistry: Classic Scientific Papers*, p 287, (Singapore: World Scientific) 2000
[2] Arfken G B, Weber H J and Harris F E 2012 *Mathematical Methods for Physicists: A comprehensive Guide* 7th edn (New York: Academic)

Chapter 7

[1] Zettili N 2009 *Quantum Mechanics* 2nd edn (West Sussex: Wiley)
[2] Cohen-Tannoudji C, Diu B and Laloë F 1977 *Quantum Mechanics* (New York: Wiley)
[3] Zare R N 1988 *Angular Momentum* (New York: Wiley)

Chapter 8

[1] Herzberg G 1950 Molecular Spectra and Molecular Structure I *Spectra of Diatomic Molecules* 2nd edn (New York: Van Nostrand Reinhold)
[2] Bransden B H and Joachain C J 2003 *Physics of Atom and Molecules* 2nd edn (Harlow: Prentice-Hall)

Chapter 9

[1] Schiff L I 1968 *Quantum Mechanics* 3rd edn (London: McGraw-Hill)
[2] Messiah A 1964 *Quantum Mechanics* (North Holland: Amsterdam)
[3] Landau L D and Lifshitz E M 1977 *Quantum Mechanics* 3rd edn (Amsterdam: Butterworth-Heinemann)
[4] Gottfried K 1998 and Ting-Mow Yan *Quantum Mechanics: Fundamentals* 2nd edn (New York: Springer)
[5] Zettili N 2009 *Quantum Mechanics* 2nd edn (West Sussex: Wiley)
[6] Weinberg S 2015 *Lectures on Quantum Mechanics* 2nd edn (Cambridge: Cambridge University Press)
[7] Rose M E 1995 *Elementary Theory of Angular Momentum* (Mineola, NY: Dover)
[8] Edmonds A R 1974 *Angular Momentum in Quantum Mechanics* 2nd edn (Princeton, NJ: Princeton University Press)
[9] Brink D M and Satchler G R 1993 *Angular Momentum* 3rd edn (Oxford: Oxford University Press)
[10] Biedenharn L C and Louck J D 2009 *Angular Momentum in Quantum Physics* (Cambridge: Cambridge University Press)
[11] Thompson W J 1994 *Angular Momentum* (New York: Wiley)
[12] Zare R N 1988 *Angular Momentum* (New York: Wiley)
[13] Chaichain M and Hagedorn R 1998 *Symmetries in Quantum Mechanics* (New York: Taylor and Francis)
[14] Varshalovich D A, Moskalev A N and Khersonskii V K 1988 *Quantum Theory of Angular Momentum* (Singapore: World Scientific)
[15] Brown J M and Carrington A 2003 *Rotational Spectroscopy of Diatomic Molecules* (Cambridge: Cambridge University Press)
[16] Lefebvre-Brion H and Field R W 2004 *The Spectra and Dynamics of Diatomic Molecules* (New York: Elsevier/Academic)

[17] Born M, Heisenberg W and Jordan P 1926 *Z. Phys.* **35** 557
Sources of Quantum Mechanics 1967 ed B L Van Der Waerden p 321 (New York: Dover)

Chapter 10

[1] Hornkohl J O and Parigger C G 2017 *Int. J. Mol. Theor. Phys.* **1** 00103
[2] Hornkohl J O and Parigger C G 2017 *Int. J. Mol. Theor. Phys.* **1** 00102
[3] Hougen J T 1962 *J. Chem. Phys.* **36** 519
[4] Larsson M 1981 *Phys. Scr.* **23** 835
[5] Zare R N 1988 *Angular Momentum* (New York: Wiley)
[6] Lefebvre-Brion H and Field R W 2004 *The Spectra and Dynamics of Diatomic Molecules* (New York: Elsevier/Academic)
[7] Brown J M and Carrington A 2003 *Rotational Spectroscopy of Diatomic Molecules* (Cambridge: Cambridge University Press)
[8] Kemble E C 2005 *The Fundamental Principles of Quantum Mechanics* (Mineola, NY: Dover)
[9] Messiah A 1964 *Quantum Mechanics* (Amsterdam: North Holland)
[10] Cohen-Tannoudji C, Diu B and Laloë F 1977 *Quantum Mechanics* (New York: Wiley)
[11] Zettili N 2009 *Quantum Mechanics* 2nd edn (West Sussex: Wiley)
[12] Gottfried K 1998 and Ting-Mow Yan *Quantum Mechanics: Fundamentals* 2nd edn (New York: Springer)
[13] Rose M E 1995 *Elementary Theory of Angular Momentum* (Mineola, NY: Dover)
[14] Edmonds A R 1974 *Angular Momentum in Quantum Mechanics* 2nd edn (Princeton, NJ: Princeton University Press)
[15] Varshalovich D A, Moskalev A N and Khersonskii V K 1988 *Quantum Theory of Angular Momentum* (Singapore: World Scientific)
[16] Landau L D and Lifshitz E M 1977 *Quantum Mechanics* 3rd edn (Amsterdam: Butterworth-Heinemann)
[17] Tung W-K 1985 *Group theory in physics* (Singapore: World Scientific)
[18] Merzbacher E 1998 *Quantum Mechanics* 3rd edn (New York: Wiley)
[19] Chaichain M and Hagedorn R 1998 *Symmetries in Quantum Mechanics* (New York: Taylor and Francis)
[20] Weinberg S 2015 *Lectures on Quantum Mechanics* 2nd edn (Cambridge: Cambridge University Press)

Chapter 11

[1] Condon E U and Shortley G 1953 *The Theory of Atomic Spectra* (Cambridge: Cambridge University Press)

Chapter 12

[1] Rose M E 1995 *Elementary Theory of Angular Momentum* (Mineola, NY: Dover)

Chapter 13

[1] ter Haar D 1946 *Phys. Rev.* **70** 222
[2] Shen Jie, Tang Tao and Wang Li-Lian 2010 Spectral Methods, Algorithms *Analysis and Applications* (Heidelberg: Springer)
[3] Greenawalt E M and Dickinson A S 1969 *J. Mol. Spectrosc.* **30** 427

[4] Chan S I and Stelman D 1963 *J. Chem Phys.* **39** 545
[5] Harris D O, Engerholm G G and Gwinn W D 1965 *J. Chem. Phys.* **43** 1515
[6] Zetik D F and Matsen F A 1967 *J. Mol. Spectrosc.* 122
[7] Dickinson A S and Certain P R 1968 *J. Chem. Phys.* 4209

Chapter 14

[1] Wallace L 1962 *Astrophys. J. Suppl. S.* **7** 165
[2] Parigger C G and Hornkohl J O 2010 *Int. Rev. At. Mol. Phys.* **1** 25
[3] Parigger C G, Woods A C, Surmick D M, Gautam G, Witte M J and Hornkohl J O 2015 *Spectrochim. Acta* B **107** 132

Chapter 15

[1] Kunze H-J 2009 *Introduction to Plasma Spectroscopy* (Heidelberg: Springer)
[2] Fujimoto T 2004 *Plasma Spectroscopy* (Oxford: Clarendon)
[3] Ochkin V N 2009 *Spectroscopy of Low Temperature Plasma* (Weinheim: Wiley)
[4] Omenetto E D 1979 *Analytical Laser Spectroscopy* (New York: Wiley)
[5] Demtröder W 2014 *Laser Spectroscopy 1: Basic Principles* 5th edn (Heidelberg: Springer)
[6] Demtröder W 2015 *Laser Spectroscopy 2: Experimental Techniques* 5th edn (Heidelberg: Springer)
[7] Hertel I V and Schulz C-P 2015 *Atoms, Molecules and Optical Physics 1, Atoms and Spectroscopy.* (Heidelberg: Springer)
[8] Hertel I V and Schulz C-P 2015 *Atoms, Molecules and Optical Physics 2, Molecules and Photons–Spectroscopy and Collisions* (Heidelberg: Springer)
[9] McKemmish L K 2021 *WIREs Comput. Mol. Sci.* **11** e1520
[10] Tennyson J *et al* 2020 *J. Quant. Spectrosc. Radiat. Transf.* **255** 107228
[11] Rothman L S, Gordon I E, Barber R J, Dothe H, Gamache R R, Goldman A, Perevalov V I, Tashkun S A and Tennyson J 2010 *J. Quant. Spectrosc. Radiat. Transf.* **111** 2139
[12] Western C M 2017 *J. Quant. Spectrosc. Radiat. Transfer* **186** 221
[13] Miziolek A W, Palleschi V and Schechter I 2006 *Laser Induced Breakdown Spectroscopy* (New York: Cambridge University Press)
[14] Singh J P and Thakur S N (ed) 2020 *Laser-Induced Breakdown Spectroscopy* 2nd edn (New York: Elsevier)
[15] De Giacomo A and Hermann J 2017 *J. Phys. D Appl. Phys.* **50** 183002
[16] Parigger C G, Surmick D M, Helstern C M, Gautam G, Bol'shakov A A and Russo R 2020 Laser Induced Breakdown *Molecular Laser-Induced Breakdown Spectroscopy. In: Laser Induced Breakdown Spectroscopy* ed J P Singh and S N Thakur 2nd edn (New York: Elsevier)
[17] C. G. Parigger. Laser-induced breakdown in gases: Experiments and simulation, in: Laser-Induced Breakdown Spectroscopy(LIBS), Fundamentals and Applications, A. W. Miziolek, V. Palleschi, I. Schechter, ed, ch 4. (New York: Cambridge University Press) 2006
[18] Parigger C G, Helstern C M, Jordan B S, Surmick D M and Splinter R 2020 *Molecules* **25** 615
[19] Parigger C G, Jordan H B S, Surmick D M and Splinter R 2020 *Molecules* **25** 988
[20] Parigger C G 2020 *Spectrochim. Acta* B **179** 106122
[21] Parigger C G, Woods A C, Surmick D M, Gautam G, Witte M J and Hornkohl J O 2015 *Spectrochim. Acta* B **107** 132

[22] Hornkohl J O, Nemes L and Parigger C G 2009 *Spectroscopy, dynamics and molecular theory of carbon plasmas and vapors. In: Advances in the Understanding of the Most Complex High-Temperature Elemental System, L. Nemes and S. Irle, ed, chapter 4* ed L Nemes and S Irle (Singapore: World Scientific) Chapter 4
[23] Parigger C G and Hornkohl J O 2020 *Quantum Mechanics of the Diatomic Molecule with Applications* (Bristol: IOP Publishing)
[24] Surmick D M and Hornkohl J O 2016 (The University of Tennessee, University of Tennessee Space Institute, Tullahoma, TN, USA) personal communication
[25] *MATLAB Release R2022a Update 5* (MA: Natick)
[26] Parigger C G, Woods A C, Witte M J, Swafford L D and Surmick D M 2014 *J. Vis. Exp.* **84** 51250
[27] Barrell H and Sears J E 1939 *Philos. Trans. Roy. Soc. London* **238** 1
[28] Ciddor P E 1996 *Appl. Opt.* **35** 1567
[29] Parigger C G, Woods A C, Surmick D M, Gautam G, Witte M J and Hornkohl J O 2015 *Spectrochim. Acta* B **107** 132
[30] Dors I G, Parigger C G and Lewis J W L 1998 *Opt. Lett.* **23** 1778
[31] Parigger C G, Plemmons D H, Hornkohl J O and Lewis J W L 1994 *J. Quant. Spectrosc. Radiat. Transf.* **52** 707
[32] Trautner S, Jasik J, Parigger C G, Pedarnig J D, Spendelhofer W, Lackner J and Veis P 2017 and *J. Heitz. Spectrochim. Acta* A **174** 331
[33] Hornkohl J O, Parigger C G and Lewis J W L 1991 *J. Quant. Spectrosc. Radiat. Transf.* **46** 405
[34] Parigger C G, Plemmons D H, Hornkohl J O and Lewis J W L 1995 *Appl. Opt.* **34** 3331
[35] Parigger C G 2022 *Foundations* **2** 934
[36] Hornkohl J O, Fleischmann J P, Surmick D M, Witte M J, Swafford L D, Woods A C and Parigger C G 2014 *J. Phys. Conf. Ser.* 548 12040
[37] Parigger C G, Woods A C, Keszler A, Nemes L and Hornkohl J O 2012 *AIP Conf. Proc.* 1464 628
[38] Woods A C, Parigger C G and Hornkohl J O 2012 *Opt. Lett.* **37** 5139
[39] Parigger C G 2023 *Foundations* **3** 1

Chapter 16

[1] Parigger C G 2006 Laser-induced breakdown in gases: experiments and simulation *Laser-Induced Breakdown Spectroscopy (LIBS), Fundamentals and Applications* ed A W Miziolek, V Palleschi and I Schechter (New York: Cambridge University Press) ch 4
[2] Parigger C G, Surmick D M, Helstern C M, Gautam G, Bol'shakov A A and Russo R 2020 Molecular laser-induced breakdown spectrosocpy *Laser-Induced Breakdown Spectroscopy* ed J P Singh and S N Thakur (New York: Elsevier Science) ch 7
[3] Parigger C G, Drake K A, Helstern C M and Gautam G 2018 *Atoms* **6** 36
[4] Hornkohl J O, Parigger C G and Lewis J W L 1991 *J. Quant. Spectrosc. Radiat. Transfer* **46** 405
[5] Parigger C G, Hornkohl J O and Nemes L 2010 *Int. J. Spectrosc.* **2010** 159382
[6] Parigger C G, Helstern C M and Gautam G 2020 *Symmetry* **12** 2116
[7] Parigger C G, Jordan H B S, Surmick D M and Splinter R 2020 *Molecules* **25** 988
[8] Kunze H-J 2009 *Introduction to Plasma Spectroscopy* (Heidelberg: Springer)
[9] Bauer D and Mulser P 2010 *High Power Laser-Matter Interaction* (Heidelberg: Springer)

[10] Hertel I V and Schulz C-P 2015 *Atoms, Molecules and Optical Physics 1, Atoms and Spectroscopy* (Heidelberg: Springer)
[11] Hertel I V and Schulz C-P 2015 *Atoms, Molecules and Optical Physics 2, Molecules and Photons—Spectroscopy and Collisions* (Heidelberg: Springer)
[12] and ed A W Miziolek, V Palleschi and I Schechter 2006 *Laser-Induced Breakdown Spectroscopy (LIBS)—Fundamentals and Applications* (New York: Cambridge University Press)
[13] Singh J P and Thakur S N (ed) 2020 *Laser-Induced Breakdown Spectroscopy* (New York: Elsevier Science)
[14] Cremers D E and Radziemski L J 2006 *Handbook of Laser-Induced Breakdown Spectroscopy* (New York: Wiley)
[15] Parigger C G, Woods A C, Witte M J, Swafford L D and Surmick D M 2014 *J. Vis. Exp.* **84** 51250
[16] Nemes L, Hornkohl J O and Parigger C G 2005 *Appl. Opt.* **44** 3686
[17] Parigger C G, Woods A C, Surmick D M, Gautam G, Witte M J and Hornkohl J O 2015 *Spectrochim. Acta* B **107** 132
[18] Hornkohl J O and Parigger C G 1996 Boltzmann equilibrium spectrum program (BESP), 1996 (accessed January 19, 2016). http://view.utsi.edu/besp/
[19] Parigger C G, Plemmons D H, Hornkohl J O and Lewis J W L 1994 *J. Quant. Spectrosc. Radiat. Transfer* **52** 707
[20] Hornkohl J O, Nemes L and Parigger C G 2009 Spectroscopy, dynamics and molecular theory of carbon plasmas and vapors *Advances in the Understanding of the Most Complex High-Temperature Elemental System* ed L Nemes and S Irle (Singapore: World Scientific) ch 4
[21] Nemes L, Keszler A M, Hornkohl J O and Parigger C G 2005 *Appl. Opt.* **44** 3661
[22] Dors I G, Parigger C G and Lewis J W L 1998 *Opt. Lett.* **23** 1778
[23] Parigger C G, Guan G and Hornkohl J O 2003 *Appl. Opt.* **42** 5986
[24] Woods A C, Parigger C G and Hornkohl J O 2012 *Opt. Lett.* **37** 5139

Chapter 17

[1] O'Keefe A and Deacon D A G 1988 *Rev. Sci. Instrum* **59** 2544
[2] Romanini D and Lehmann K K 1993 *J. Chem. Phys.* **99** 6287
[3] Huestis D L, Copeland R A, Knutsen K, Slanger T G, Jongma R T, Boogaarts M G H and Meijer G 1994 *Can. J. Phys.* **72** 1109
[4] Scherer J J, Paul J B, Collier C P and Saykally R J 1995 *Chem. Phys. Lett.* **102** 5190
[5] O'Keefe A, Scherer J J, Cooksy A L, Sheeks R, Heath J and Saykally R J 1990 *Chem. Phys. Lett.* **172** 214
[6] Jongma R T, Boogaarts M G H, Holleman I and Meijer G 1995 *Rev. Sci. Instrum.* **66** 2821
[7] Yu T and Lin M C 1993 *J. Am. Chem. Soc.* **115** 4371
[8] Yu T and Lin M C 1994 *J. Phys. Chem.* **98** 9697
[9] Cheskis S 1995 *J. Chem. Phys.* **102** 1851
[10] Zalicki P, Ma Y, Zare R N, Wahl E H, Dadamino J R, Owano T G and Kruger C H 1995 *Chem. Phys. Lett.* **234** 269
[11] Meijer G, Boogaarts M G H, Jongma R T, Parker D H and Wodtke A M 1994 *Chem. Phys. Lett.* **217** 112
[12] Wang C-C, Nemes L and Lin K-C 1995 *Chem. Phys. Lett.* **245** 585
[13] Nemes L and Szalay P G 1999 *Models Chem.* **136** 205

[14] Szalay P G and Nemes L 1999 *Molec. Phys.* **96** 359
[15] Hornkohl J O, Nemes L and Parigger C G 2009 Spectroscopy, dynamics and molecular theory of carbon plasmas and vapors *Advances in the Understanding of the Most Complex High-Temperature Elemental* ed L Nemes and S Irle (Singapore: World Scientific) ch 4
[16] Parigger C G and Hornkohl J O 2020 *Quantum Mechanics of the Diatomic Molecule with Applications* (Bristol: IOP Publishing)
[17] Parigger C G 2023 *Foundations* **3** 1
[18] Parigger C G, Surmick D M, Helstern C M, Gautam G, Bol'shakov A A and Russo R 2020 Molecular laser-induced breakdown spectroscopy *Laser Induced Breakdown Spectroscopy* ed J P Singh and S N Thakur 2nd edn (New York: Elsevier)
[19] Brzozowksi J, Bunker P, Elander N and Erman P 1976 *Astrophys. J.* **207** 414
[20] Erman P 1979 Astrophysical applications of time resolved spectroscopy of small molecules *Molecular Spectroscopy Volume 6: A Review of the Literature published in 1977 and 1978* ed R F Barrow, D A Long and J Sheridian (London: The Royal Society Chemistry)
[21] Erman P 1979 *Phys. Scr.* **20** 575
[22] Warnatz J 1984 *Combustion Chemistry* (New York: Springer)
[23] Raiche G A and Jeffries J B 1993 *Appl. Opt.* **32** 4629
[24] Engeln R, Letourneur K G Y, Boogarts M G H, van den Sanden M C M and Schram D C 1999 *Chem. Phys. Lett.* **310** 405
[25] Ubachs W, Meijer G, ter Meulen J J and Dymanus A 1986 *J. Chem. Phys.* **84** 3032
[26] Parigger C G, Woods A C, Surmick D M, Gautam G, Witte M J and Hornkohl J O 2015 *Spectrochim. Acta* B **107** 132
[27] *MATLAB Release R2022a Update 5* (Natick, MA: The MathWorks, Inc)
[28] Surmick D M and Hornkohl J O 2016 (The University of Tennessee, University of Tennessee Space Institute, Tullahoma, TN, USA) personal communication
[29] Hornkohl J O 2004 Private communication, The University of Tennessee, University of Tennessee Space Institute, Tullahoma, TN, USA
[30] Nemes L and Parigger C G 2023 *Foundations* **3** 16
[31] Luque J and Crosley D R 1999 *LIFBASE, Database and spectral simulation for diatomic molecules (v 1.6)* (Menlo Park, CA: SRI International) SRI International Report MP-99-009
[32] Luque J and Crosley D R 2021 *LIFBASE: Database and Spectral Simulation for Diatomic Molecules* (Menlo Park, CA: SRI International)
[33] Luque J and Crosley D R 1996 *J. Chem. Phys.* **104** 2146
[34] Luque J and Crosley D R 1996 *J. Chem. Phys.* **104** 3907
[35] Tennyson J *et al* 2020 *J. Quant. Spectrosc. Radiat. Transf.* **255** 107228
[36] Masseron T, Plez B, Van Eck S, Colin R, Daoutidis I, Godefroid M, Coheurand P-F, Bernath P, Jorissen A and Christlieb N 2014 *Astron. Astrophys.* **571**
[37] Furtenbacher T, Hegedus S T, Tennyson T and Császár A G 2022 *Phys. Chem. Chem. Phys.* **24** 19287

Chapter 18

[1] Hornkohl J O, Parigger C G and Lewis J W L 1991 *J. Quant. Spectrosc. Radiat. Transfer* **46** 405
[2] Parigger C G, Helstern C M and Gautam G 2019 *Atoms* **7** 7030074

[3] Gordon S and McBride B J 1976 Computer program for calculation of complex equilibrium compositions, rocket performance, incident and reflected shocks, and chapman- jouguet detonations *NASA Lewis Research Center, Interim Revision, NASA Report SP-273* **273**
[4] McBride B J and Gordon S 2005 *Computer Program for Calculating and Fitting Thermodynamic Functions, NASA RP-1271* **1271** 1271
[5] Parigger C G, Hornkohl J O and Nemes L 2010 *Int. J. Spectrosc.* **2010** 159382
[6] Hornkohl J O and Parigger C G 1996 Boltzmann equilibrium spectrum program (BESP), 1996 (accessed January 19, 2016). http://view.utsi.edu/besp/.
[7] Nemes L, Keszler A M, Hornkohl J O and Parigger C G 2005 *Appl. Opt.* **44** 3661
[8] Park H S, Nam S H and Park S M 2005 *J. Appl. Phys.* **2005** 113103
[9] Parigger C G, Woods A C, Surmick D M, Gautam G, Witte M J and Hornkohl J O 2015 *Spectrochim. Acta* B **107** 132
[10] Nelder J A and Mead R 1965 *Comput. J.* **7** 308
[11] Salieri F, Quarteroni A and Sacco R 2000 *Numerical Mathematics.* (New York: Springer)
[12] Luque J and Crosley D R 1999 *LIFBASE, Database and spectral simulation for diatomic molecules (v 1.6* (Menlo Park, CA: SRI International) SRI International Report MP-99-009
[13] Western C M 2017 *J. Quant. Spectrosc. Radiat. Transfer* **186** 221
[14] Western C M 2019 Private communication
[15] Downs M J and Birch K B 1994 *Metrologia* **31** 315
[16] Parigger C G 2006 Laser-induced breakdown in gases: experiments and simulation *Laser-Induced Breakdown Spectroscopy (LIBS), Fundamentals and Applications* ed A W Miziolek, V Palleschi and I Schechter (New York: Cambridge University Press) ch 4
[17] Kroll N and Watson K M 1972 *Phys. Rev.* A **5** 1883
[18] Thiyagarajan M and Thompson S 2012 *J. Appl. Phys.* **111** 073302
[19] Gautam G, Helstern C M, Drake K A and Parigger C G 2016 *Int. Rev. At. Mol. Phys.* **7** 45
[20] Parigger C G, Helstern C M, Drake K A and Gautam G 2017 *Int. Rev. At. Mol. Phys.* **8** 53
[21] Helstern C M and Parigger C G 2019 *J. Phys.: Conf. Ser.* **1289** 012016
[22] Parigger C G, Surmick D M, Helstern C M, Gautam G, Bol'shakov A A and Russo R 2020 Molecular laser-induced breakdown spectrosocpy *Laser-Induced Breakdown Spectroscopy* ed J P Singh and S N Thakur (New York: Elsevier Science) ch 7
[23] Parigger C G, Woods A C, Witte M J, Swafford L D and Surmick D M 2014 *J. Vis. Exp.* **84** 51250
[24] Griem H 1974 *Spectral Line Broadening by Plasma* (New York: Academic)
[25] Konjević N 2002 *J. Phys. Chem. Ref. Data* **31** 819
[26] Parigger C G 2019 *Atoms* **7** 7030061
[27] Parigger C G 2019 *Contr. Astron. Obs. Skalnaté Pleso* **50** accepted

Chapter 19

[1] Roth K C, Meyer D M and Hawkins I 1993 *Astrophys. J.* **413** L67
[2] Leach S 2004 *Can. J. Chem.* **82** 730
[3] Ram R S, Davis S P, Wallace L, Englman R, Appadoo D R T and Bernath P F 2006 *J. Mol. Spectrosc.* **237** 225
[4] Brooke J S A, Ram R S, Western C M, Li G, Schwenke D W and Bernath P F 2014 *Astrophys. J. Suppl. Ser.* **210** 1
[5] Davis S P 1987 *Publ. Astron. Soc. Pac.* **99** 1105
[6] Kunze H-J 2009 *Introduction to Plasma Spectroscopy* (Heidelberg: Springer)

[7] Fujimoto T 2004 *Plasma Spectroscopy* (Oxford: Clarendon)
[8] Ochkin V N 2009 *Spectroscopy of Low Temperature Plasma* (Weinheim: Wiley)
[9] Demtröder W 2014 *Laser Spectroscopy 1: Basic Principles* 5th edn (Heidelberg: Springer)
[10] Demtröder W 2015 *Laser Spectroscopy 2: Experimental Techniques* 5th edn (Heidelberg: Springer)
[11] Miziolek A W, Palleschi V and Schechter I 2006 *Laser Induced Breakdown Spectroscopy* (New York: Cambridge University Press)
[12] Singh J P and Thakur S N (ed) 2007 *Laser-Induced Breakdown Spectroscopy* (Amsterdam: Elsevier Science)
[13] Tennyson J *et al* 2020 *J. Quant. Spectrosc. Radiat. Transf.* **255** 107228
[14] Luque J and Crosley D R 2021 *LIFBASE: Database and Spectral Simulation for Diatomic Molecules* (Menlo Park, CA: SRI International)
[15] Western C M 2017 *J. Quant. Spectrosc. Radiat. Transfer* **186** 221
[16] McKemmish L K 2021 *WIREs Comput. Mol. Sci.* **11** e1520
[17] Rothman L S, Gordon I E, Barber R J, Dothe H, Gamache R R, Goldman A, Perevalov V I, Tashkun S A and Tennyson J 2010 *J. Quant. Spectrosc. Radiat. Transf.* **111** 2139
[18] *MATLAB Release R2022a Update 5* (MA: Natick)
[19] Parigger C G and Hornkohl J O 2020 *Quantum Mechanics of the Diatomic Molecule with Applications* (Bristol: IOP Publishing)
[20] Parigger C G 2023 *Foundations* **3** 1
[21] Hornkohl J O, Parigger C G and Lewis J W L 1991 *J. Quant. Spectrosc. Radiat. Transfer* **46** 405
[22] Dunham J L 1932 *Phys. Rev.* **41** 721
[23] *National Institute of Standards and Technology (NIST) Chemistry WebBook, SRD 69, for the Cyano Radical, Constants of Diatomic Molecules*. 2021
[24] Whiting E E 1995 Private communication
[25] Whiting E E, Park C, Liu Y, Arnold J and Paterson J 1996 *NEQAIR96, Nonequilibrium and Equilibrium Radiative Transport and Spectra Program: User's Manual* (CA: NASA Ames Research Center) Technical Report NASA RP-1389
[26] Boulous P M I and Pfender E 1994 *Thermal Plasmas–Fundamentals and Applications* (New York: Plenum)
[27] McBride B and Gordan S 1994 *Interim Revision NASA Report RP-1311 Part* I (Cleveland, OH: NASA Lewis Research Center)
[28] McBride B and Gordan S 1996 *Interim Revision NASA Report RP-1311 Part II* (Cleveland, OH: NASA Lewis Research Center)
[29] Laux C O 2002 Radiation and nonequilibrium collisional-radiative models, von Karman Institute Lecture Series 2002-07 *Physico-Chemical Modeling of High Enthalpy and Plasma Flows* ed D Fletcher, J M Charbonnier, G S R Sarma and T Magin (Flanders: Rhode-Saint-Genèse))
[30] Syme A-M and McKemmish L K 2020 *Mon. Not. R. Astron. Soc.* **499** 25
[31] Syme A-M and McKemmish L K 2021 *Mon. Not. R. Astron. Soc.* **505** 4383
[32] Western C M 2019 Private communication
[33] Condon E U and Shortley G 1953 *The Theory of Atomic Spectra* (Cambridge: Cambridge University Press)
[34] Hilborn R C 1982 *Am. J. Phys.* **50** 982 http://arxiv.org/ftp/physics/papers/0202/0202029.pdf
[35] Thorne A P 1988 *Spectrophysics* 2nd edn (London: Chapman and Hall)

[36] Parigger C G 2023 *Atoms* **11** 62
[37] Whiting E E 1968 *J. Quant. Spectrosc. Radiat. Transf.* **8** 1379
[38] Parigger C G and Hornkohl J O 2020 *Quantum Mechanics of the Diatomic Molecule with Applications* (Bristol: IOP Publishing)

Chapter 20

[1] Hornkohl J O, Nemes L and Parigger C G 2009 Spectroscopy, dynamics and molecular theory of carbon plasmas and vapors *Advances in the Understanding of the Most Complex High-Temperature Elemental System* ed L Nemes and S Irle (Singapore: World Scientific) ch 4
[2] Witte M J and Parigger C G 2014 *J. Phys.: Conf. Ser.* 548 012052
[3] Parigger C G, Woods A C and Rezaee M R 2012 *J. Phys.: Conf. Ser.* 397 012022
[4] Parigger C G 2013 *Spectrochim. Acta* B **78-79** 4
[5] De Lucia F C, Harmon R S, McNesby K L, Winkel R J and Miziolek A W 2003 *Appl. Opt.* **42** 6148
[6] Parigger C G, Plemmons D H, Hornkohl J O and Lewis J W L 1994 *J. Quant. Spectrosc. Radiat. Transfer* **52** 707
[7] Witte M J, Parigger C G, Bullock N A, Merten J A and Allen S D 2014 *Appl. Spectrosc.* **68** 367
[8] Witte M J and Parigger C G 2013 *Int. Rev. At. Mol. Phys.* **4** 63
[9] Parigger C G, Woods A C, Witte M J, Swafford L D and Surmick D M 2014 *J. Vis. Exp.* **84** 51250
[10] Parigger C G, Hornkohl J O, Keszler A M and Nemes L 2003 *Appl. Opt.* **42** 6192
[11] Nemes L, Keszler A M, Hornkohl J O and Parigger C G 2005 *Appl. Opt.* **44** 3661
[12] Woods A C, Parigger C G and Hornkohl J O 2012 *Opt. Lett.* **37** 5139
[13] Parigger C G, Woods A C, Surmick D M, Gautam G, Witte M J and Hornkohl J O 2015 *Spectrochim. Acta* B **107** 132
[14] Gornushkin I B, Merk S, Demidov A, Panne U, Shabanov S V, Smith B W and Omenetto N 2012 *Spectrochim. Acta* B **76** 203
[15] Parigger C G and Oks E 2010 *Int. Rev. At. Mol. Phys.* **1** 13
[16] Parigger C G 2010 *Int. Rev. At. Mol. Phys.* **1** 129
[17] Parigger C G, Woods A C and Hornkohl J O 2011 *Int. Rev. At. Mol. Phys.* **2** 77
[18] Parigger C G, Dackman M and Hornkohl J O 2008 *Appl. Opt.* **47** G1
[19] Parigger C G, Woods A C and Hornkohl J O 2012 *Appl. Opt.* **51** B1
[20] Aragón C and Aguilera J A 2010 *Spectrochim. Acta* B **65** 395
[21] Sherbini A M E L, Hegazy H and Sherbini T M E L 2006 *Spectrochim. Acta* B **61** 532
[22] Detalle V, Heón R and Sabsabi M 2001 *Spectrochim. Acta* B **56** 1011
[23] Griem H 1974 *Spectral Line Broadening by Plasma* (New York: Academic)
[24] Konjević N 1999 *Phys. Rep.* **316** 339
[25] Chen F F 1995 *Introduction to Plasma Physics* (New York: Springer)
[26] Cristoforetti G, De Giacomo A, Dell'Aglio M, Legnaioli S, Tognoni E, Palleschi V and Omenetto N 2010 *Spectrochim. Acta* B **65** 86
[27] Djurović S, Ćirišan M, Demura A V, Demchenko G V, Nikolić D, Gigosos M A and González M Á 2009 *Phys. Rev.* E **79** 046402
[28] Oks E, Parigger C G and Plemmons D H 2003 *Appl. Opt.* **42** 5992
[29] Schrödinger E 1926 *Ann. Phys.* **385** 437
[30] Schrödinger E 1926 *Phys. Rev.* **28** 1049

[31] Laux C 2003 *Plasma Sources Sci. Technol.* **12** 125
[32] Oks E 2006 *Stark Broadening of Hydrogen and Hydrogenlike Spectral Lines on Plasmas: The Physical Insight* (Oxford: Alpha Science International)
[33] Camacho J J, Díaz L, Santos M and Poyato J M L 2011 *Spectrochim. Acta* B **66** 57
[34] Parigger C G, Hornkohl J O and Nemes L 2007 *Appl. Opt.* **46** 4026
[35] Kim J-H and Lee H-J 2006 *J. Korean Phys. Soc.* **49** 3S184
[36] Aydin Ü, Roth P, Gehlen C D and Noll R 2008 *Spectrochim. Acta* B **63** 1060
[37] Gornushkin I B, Shabanov S V, Merk S, Tognoni E and Panne U 2010 *J. Anal. Atom. Spectrom.* **25** 1643
[38] Cremers D E and Radziemski L J 2006 *Handbook of Laser-Induced Breakdown Spectroscopy* (New York: Wiley)

Chapter 21

[1] Pretty W E 1927 *Proc. Phys. Soc.* 40 71
[2] Johnson R C 1927 *Phil. Trans. Royal Soc.* A **226** 157
[3] Phillips J G and Davis S P 1968 *The Berkeley Analysis of Molecular Spectra, Vol. 2, I. The Swan System of the C_2 Molecule* (Berkeley, CA: University of California Press)
[4] Parigger C G, Plemmons D H, Hornkohl J O and Lewis J W L 1994 *J. Quant. Spectrosc. Radiat. Transfer* **52** 707
[5] Dufour P, Blouin S, Coutu S, Fortin-Archambault M, Thibeault C, Bergeron P and Fontaine G 2017 *The Montreal White Dwarf Database: A Tool for the Community. In: Astronomical Society of the Pacific (ASP) Conf. Series 509, Proc. 20th European White Dwarf Workshop*; P-E Tremblay, B Gaensicke and T Marsh (San Francisco, CA, USA: Astronomical Society of the Pacific) Available online: http://dev.montrealwhitedwarfdatabase.org
[6] Parigger C G, Helstern C M, Gautam G and Drake D A 2019 *J. Phys.: Conf. Ser.* 1289 012001
[7] Hornkohl J O, Nemes L and Parigger C G 2009 *Spectroscopy, dynamics and molecular theory of carbon plasmas and vapors. In: Advances in the Understanding of the Most Complex High-Temperature Elemental System* ed L Nemes and S Irle (Singapore: World Scientific) ch 4
[8] Parigger C G 2023 *Foundations* **3** 1
[9] Parigger C G and Hornkohl J O 2020 *Quantum Mechanics of the Diatomic Molecule with Applications* (Bristol: IOP Publishing)
[10] Tennyson J *et al* 2020 *J. Quant. Spectrosc. Radiat. Transf.* **255** 107228
[11] Ochkin V N 2009 *Spectroscopy of Low Temperature Plasma* (Weinheim: Wiley)
[12] Kunze H-J 2009 *Introduction to Plasma Spectroscopy* (Heidelberg: Springer)
[13] Fujimoto T 2004 *Plasma Spectroscopy* (Oxford: Clarendon)
[14] Demtröder W 2014 *Laser Spectroscopy 1: Basic Principles* 5th edn (Heidelberg: Springer)
[15] Demtröder W 2015 *Laser Spectroscopy 2: Experimental Techniques* 5th edn (Heidelberg: Springer)
[16] Miziolek A W, Palleschi V and Schechter I 2006 *Laser Induced Breakdown Spectroscopy* (New York: Cambridge University Press)
[17] Singh J P and Thakur S N (ed) 2020 *Laser-Induced Breakdown Spectroscopy* 2nd edn (New York: Elsevier)
[18] Western C M 2017 *J. Quant. Spectrosc. Radiat. Transfer* **186** 221
[19] McKemmish L K 2021 *WIREs Comput. Mol. Sci.* **11** e1520

[20] *MATLAB Release R2022a Update 5* (MA: Natick)
[21] Nelder J A and Mead R 1965 *Comp. J.* **7** 308
[22] Wigmer E and Witmer E E 1928 *Z. Phys.* **51** 859
[23] Hettema E H 2000 *On the Structure of the Spectra of Two-Atomic Molecules According to Quantum Mechanics. In: Quantum Chemistry: Classic Scientific Papers* (Singapore: World Scientific)
[24] Yurchenko S N, Szabo I, Pyatenko E and Tennyson J J 2018 *Mon. Notices Royal Astron. Soc.* **480** 3397
[25] McKemmish L K, Syme A-M, Borsovszky J, Yurchenko S N, Tennyson J, Furtenbacher T and Császár A G 2020 *Mon. Notices Royal Astron. Soc.* **497** 1081
[26] Parigger C G 2023 *Atoms* **11** 62
[27] Condon E U and Shortley G 1953 *The Theory of Atomic Spectra* (Cambridge: Cambridge University Press)
[28] Hilborn R C 1982 *Am. J. Phys.* **50** 982
[29] Thorne A P 1988 *Spectrophysics* 2nd edition (London: Chapman and Hall)
[30] Ciddor P E 1996 *Appl. Opt.* **35** 1567
[31] Corney A 1977 *Atomic and Laser Spectroscopy* (Oxford: Clarendon)
[32] Parigger C G 2023 *Preprints* **2023** 2023050423
[33] Hornkohl J O, Parigger C G and Lewis J W L 1996 On the use of line strengths in applied diatomic spectroscopy *Technical Digest Series of the Laser Applications to Chemical and Environmental Analysis Conf.* (Washington, DC: Optica Publishing Group)
[34] Suzuki T, Saito S and Hirota E 1985 *J. Molec. Spectrosc.* **113** 399

Chapter 22

[1] Dors I G, Parigger C G and Lewis J W L 1998 *Opt. Lett.* **23** 1778
[2] Surmick D M and Parigger C G 2014 *J. Phys.: Conf. Ser.* 548 012046
[3] Bransden B H and Joachain C J 2003 *Physics of Atoms and Molecules* 2nd edn (New York: Prentice-Hall)
[4] Piehler T N, DeLucia F C, Munson C A, Homan B E, Miziolek A W and McNesby K L 2005 *Appl. Opt.* **44** 3654
[5] De Lucia F C, Harmon R S, McNesby K L, Winkel R J and Miziolek A W 2003 *Appl. Opt.* **42** 6148
[6] Sabsabi M and Cielo P 1995 *Appl. Spectrosc.* **44** 3654
[7] Rai A K, Yueh F and Signh J P 2003 *Appl. Opt.* **42** 2078
[8] Lightstone J M, Carney J R, Boswel C J and Wilikinson J 2007 *AIP Conf. Proc.* **955** 1255
[9] Parigger C G, Hornkohl J O and Nemes L 2007 *Appl. Opt.* **46** 4026
[10] Surmick D M and Parigger C G 2014 *Appl. Spectrosc.* **68** 992
[11] Parigger C G, Woods A C, Witte M J, Swafford L D and Surmick D M 2014 *J. Vis. Exp.* **84** 51250
[12] Nelder J A and Mead R 1965 *Comput. J.* **7** 308
[13] Lagarias J C, Reeds J A, Wright M H and Wright P E 1998 *SIAM J. Optim.* **9** 112
[14] Parigger C G and Hornkohl J O 2011 *Spectrochim. Acta* A **81** 403
[15] Nemes L, Hornkohl J O and Parigger C G 2005 *Appl. Opt.* **44** 3686
[16] Konjević N, Ivković M and Sakan N 2012 *Spectrochim. Acta* B **76** 16
[17] Ispolatov Y and Oks E 1994 *J. Quant. Spectrosc. Radiat. Transfer* **51** 129
[18] Oks E, Parigger C G and Plemmons D H 2003 *Appl. Opt.* **42** 5992

[19] Parigger C G 2006 *AIP Conf. Proc.* **874** 101
[20] Parigger C G, Gautam G, Woods A C, Surmick D M and Hornkohl J O 2014 *Trends Appl. Spectrosc.* **11** 1

Chapter 23

[1] Dors I G, Parigger C G and Lewis J W L 1998 *Opt. Lett.* **23** 1778
[2] Surmick D M and Parigger C G 2014 *Appl. Spectrosc.* **68** 992
[3] Parigger C G, Woods A C, Surmick D M, Donaldson A B and Height J L 2014 *Appl. Spectrosc.* **68** 362
[4] Parigger C G and Hornkohl J O 2011 *Spectrochim. Acta* A **81** 404
[5] Parigger C G 2023 *Foundations* **3** 1
[6] Parigger C G and Hornkohl J O 2020 *Quantum Mechanics of the Diatomic Molecule with Applications* (Bristol: IOP Publishing)
[7] Tennyson J *et al* 2020 *J. Quant. Spectrosc. Radiat. Transf.* **255** 107228
[8] Parigger C G 2022 *Int. Rev. At. Mol. Phys.* **14** 7
[9] Kunze H-J 2009 *Introduction to Plasma Spectroscopy* (Heidelberg: Springer)
[10] Fujimoto T 2004 *Plasma Spectroscopy* (Oxford: Clarendon)
[11] Ochkin V N 2009 *Spectroscopy of Low Temperature Plasma* (Weinheim: Wiley)
[12] Demtröder W 2014 *Laser Spectroscopy 1: Basic Principles* 5th edn (Heidelberg: Springer)
[13] Demtröder W 2015 *Laser Spectroscopy 2: Experimental Techniques* 5th edn (Heidelberg: Springer)
[14] Miziolek A W, Palleschi V and Schechter I (ed) 2006 *Laser-Induced Breakdown Spectroscopy (LIBS)—Fundamentals and Applications* (New York: Cambridge University Press)
[15] Singh J P and Thakur S N (ed) 2007 *Laser-Induced Breakdown Spectroscopy* (Amsterdam: Elsevier Science)
[16] Western C M 2017 *J. Quant. Spectrosc. Radiat. Transfer* **186** 221
[17] McKemmish L K 2021 *WIREs Comput. Mol. Sci.* **11** e1520
[18] Rothman L S, Gordon I E, Barber R J, Dothe H, Gamache R R, Goldman A, Perevalov V I, Tashkun S A and Tennyson J 2010 *J. Quant. Spectrosc. Radiat. Transf.* **111** 2139
[19] *MATLAB Release R2022a Update 5* (Natick, MA: The MathWorks, Inc.)
[20] Nelder J A and Mead R 1965 *Comp. J.* **7** 308
[21] Patrascu A T, Yurchenko S N and Tennyson J 2015 *Mon. Notices Royal Astron. Soc.* **449** 3613
[22] Bowesman C A, Shuai M and Yurchenko S N 2021 *Mon. Notices Royal Astron. Soc.* **508** 3181
[23] Condon E U and Shortley G 1953 *The Theory of Atomic Spectra* (Cambridge: Cambridge University Press)
[24] Hilborn R C 1982 *Am. J. Phys.* **50** 982 http://arxiv.org/ftp/physics/papers/0202/0202029.pdf
[25] Thorne A P 1988 *Spectrophysics* 2nd edition (London: Chapman and Hall)
[26] Wigner E and Witmer E E 1928 *Z. Phys.* **51** 859
Hettema H 2000 *Quantum Chemistry: Classic Scientific Papers* (Singapore: World Scientific) p 287
[27] Hettema E H 2000 *On the Structure of the Spectra of Two-Atomic Molecules According to Quantum Mechanics. In: Quantum Chemistry: Classic Scientific Papers* (Singapore: World Scientific)
[28] Parigger C G 2023 *Preprints* **2023** 2023050423

Chapter 24

[1] Levin D A, Laux C O and Kruger C H 1999 *J. Quant. Spectrosc. Radiat. Transfer* **61** 377
[2] Crosley D R and Jeffries J B 1996 Temperature measurements by laser-induced fluorescence of the hydroxyl radical *Temperature: Its Measurement and Control in Science and Industry* ed L J F Schooley vol 6 (New York: American Institute of Physics)
[3] Battles B E and Hanson R K 1995 *J. Quant. Spectrosc. Radiat. Transfer* **54** 521
[4] Levin D A, Laux C O and Laux C H 1995 A general model for the spectral calculation of oh radiation in the ultraviolet *AIAA paper 95-1990 presented at the 26th AIAA Plasmadynamics and Lasers Conf.(June 19-22, 1995) (San Diego, CA)*
[5] Laoux C O 1993 Optical diagnostics and radiative emission of air plasmas *PhD Dissertation* Department of Mechanical Engineering. Stanford University, Stanford, CA
[6] Rakestraw D J, Farrow R L and Dreier T 1990 *Opt. Lett.* **15** 709
[7] Kohse-Höinghaus K, Meier U and Attal-Tretout B 1990 *Appl. Opt.* **29** 1560
[8] Attal-Tretout B, Schmidt S C, Crete E, Dumas P and Taran J P 1990 *J. Quant. Spectrosc. Radiat. Transfer* **43** 351
[9] Desgroux P and Cottereau M J 1991 *Appl. Opt.* **30** 90
[10] Ewart P and Kaczmarek M 1991 *Appl. Opt.* **30** 3996–9
[11] Cignoli F, Benecchi S and Zizak G 1992 *Opt. Lett.* **17** 229
[12] Nyholm K, Maier R, Aminoff C G and Kaivola M 1993 *Appl. Opt.* **32** 919
[13] Nyholm K, Fritzon R and Alden M 1993 *Opt. Lett.* **18** 1672
[14] Seitzman J M, Hanson R K, Debarber P A and Hess C F 1994 *Appl. Opt.* **33** 4000
[15] Rahn L A and Brown M S 1994 *Opt. Lett.* **19** 1249
[16] Allen M G, McManus K R, Sonnenfroh D M and Paul P H 1995 *Appl. Opt.* **34** 6287
[17] Palmer J L and Hanson R K 1996 *Appl. Opt.* **35** 485
[18] Neuber A A, Janicka J and Hassel E P 1996 *Appl. Opt.* **35** 4033
[19] Parigger C G, Lewis J W L, Plemmons D P and Hornkohl J O 1996 Nitric oxide optical breakdown spectra and analysis by the use of the program NEQAIR *Laser Appl. Chem. Bio. Env. Anal.* **3** 85
[20] Parigger C G, Guan G and Hornkohl J O 2003 *Appl. Opt.* **42** 5986
[21] Tellinghuisen J 1972 *J. Mol. Spectrosc.* **44** 194
[22] Tellinghuisen J 1974 *J. Comput. Phys.* **6** 221
[23] Zare R N, Schmeltekopf A L, Harrop W J and Albritton D L 1973 *J. Mol. Spectrosc.* **46** 37
[24] Tatum J B 1967 The interpretation of intensities in diatomic molecular spectra *Astrophys. J. Suppl.* **XIV** 21
[25] Hornkohl J O, Parigger C G and Lewis J W L 1991 *J. Quant. Spectrosc. Radiat. Transfer* **46** 405
[26] Hornkohl J O and Parigger C G 1996 *Am. J. Phys.* **64** 623
[27] Dieke G H and Crosswhite H M 1962 *J. Quant. Spectrosc. Radiat. Transfer* **2** 97
[28] Coxon J A 1980 *Can. J. Phys.* **58** 933
[29] Coxon J A and Foster S C 1981 *Can. J. Phys.* **60** 41
[30] Coxon J A, Sappey A D and Copeland R A 1991 *J. Mol. Spectrosc.* **145** 41
[31] Nelder J A and Mead R 1965 *Comput. J.* **7** 308
[32] Salieri F, Quarteroni A and Sacco R 2000 *Numerical Mathematics* (New York: Springer)

Chapter 25

[1] Wigner E and Witmer E E 1928 *Z. Phys.* **51** 859
Hettema H 2000 *Quantum Chemistry: Classic Scientific Papers* (Singapore: World Scientific) p 287
[2] Hettema E H 2000 *On the Structure of the Spectra of Two-Atomic Molecules According to Quantum Mechanics. In: Quantum Chemistry: Classic Scientific Papers* (Singapore: World Scientific)
[3] Parigger C G 2023 *Foundations* **3** 1
[4] Parigger C G, Guan G and Hornkohl J O 2003 *Appl. Opt.* **42** 5986
[5] Tennyson J *et al* 2020 *J. Quant. Spectrosc. Radiat. Transf* **255** 107228
[6] Brooke J S A, Bernath P F, Western C M, Sneden C, Afşar M M, Li G and Gordon I E 2016 *J. Quant. Spectrosc. Radiat. Transf* **138** 142
[7] Yousefi M, Bernath P F, Hodges J and Masseron T 2018 *J. Quant. Spectrosc. Radiat. Transf.* **217** 416
[8] Bernath P F 2020 *J. Quant. Spectrosc. Radiat. Transf.* **240** 106687
[9] Rothman L S, Gordon I E, Barber R J, Dothe H, Gamache R R, Goldman A, Perevalov V I, Tashkun S A and Tennyson J 2010 *J. Quant. Spectrosc. Radiat. Transf.* **111** 2139
[10] Luque J and Crosley D R 2021 *LIFBASE: Database and Spectral Simulation for Diatomic Molecules* (Menlo Park, CA: SRI International)
[11] Luque J and Crosley D R 1998 *J. Chem. Phys.* **109** 439
[12] Tatum J *Stellar Atmospheres* Open Education Resource LibreTexts Project: LibreTexts Physics, shared under CC BY-NC 4.0 licence, University of Victoria, BC, Canada

Chapter 26

[1] Kunze H-J 2009 *Introduction to Plasma Spectroscopy* (Heidelberg: Springer)
[2] Fujimoto T 2004 *Plasma Spectroscopy* (Oxford: Clarendon)
[3] Ochkin V N 2009 *Spectroscopy of Low Temperature Plasma* (Weinheim: Wiley)
[4] Boulous M I, Fauchais P and Pfender E 1994 *Thermal Plasmas–Fundamentals and Applications* (New York: Plenum)
[5] Cremers D E and Radziemski L J 2006 *Handbook of Laser-Induced Breakdown Spectroscopy* (New York: Wiley)
[6] Miziolek A W, Palleschi V and Schechter I 2006 *Laser Induced Breakdown Spectroscopy* (New York: Cambridge University Press)
[7] Singh J P and Thakur S N (ed) 2020 *Laser-Induced Breakdown Spectroscopy* 2nd edn (New York: Elsevier)
[8] De Giacomo A and Hermann J 2017 *J. Phys. D: Appl. Phys.* **50** 183002
[9] Fatima H, Ullah M U, Ahmad S, Imran M, Sajjad S, Hussain S and Qayyum A 2021 *Springer Nature Appl. Sci.* **3** 646
[10] Chen Y-L and Lewis J W L L 2001 *Opt. Express* **9** 360
[11] Qin W, Chen Y-L and Lewis J W L 2005 *International Flame Research Foundation (IFRF) Combust. J.* 200508
[12] Parigger C G, Jordan H B S, Surmick D M and Splinter R 2020 *Molecules* **25** 988
[13] Parigger C G, Guan G and Hornkohl J O 2003 *Appl. Opt.* **42** 5986
[14] Parigger C G 2022 *Int. Rev. At. Mol. Phys.* **13** 15
[15] Rai A K, Pati J K, Parigger C G and Rai A K 2019 *Atoms* **7** 72

[16] McBride B J and Gordon S 2005 *Computer Program for Calculating and Fitting Thermodynamic Functions, NASA RP-1271* **1271**
[17] Parigger C G and Helstern C M 2023 *J. Phys.: Conf. Ser.* **2439** 012004
[18] Parigger C G, Helstern C M, Jordan B S, Surmick D M and Splinter R 2020 *Molecules* **25** 615
[19] Parigger C G 2020 *Spectrochim. Acta* B **179** 106122

Chapter 27

[1] Woods A C, Parigger C G and Hornkohl J O 2012 *Opt. Lett.* **37** 5139
[2] Woods A C and Parigger C G 2014 *J. Phys.: Conf. Ser.* **548** 012037
[3] Parigger C G, Woods A C, Witte M J, Swafford L D and Surmick D M 2014 *J. Vis. Exp.* **84** 51250
[4] Amoruso S, Bruzzese R, Spinelli N and Velotta R 1997 *J. Phys.* B **36** 3227
[5] Parigger C G and Oks E 2010 *Int. Rev. At. Mol. Phys.* **1** 13
[6] Hornkohl J O, Nemes L and Parigger C G 2009 *Spectroscopy, dynamics and molecular theory of carbon plasmas and vapors. In: Advances in the Understanding of the Most Complex High-Temperature Elemental System* ed L Nemes and S Irle (Singapore: World Scientific) Chapter 4
[7] Witte M J, Parigger C G, Bullock N A, Merten J A and Allen S D 2014 *Appl. Spectrosc.* **68** 367
[8] Parigger C G, Swafford L D, Woods A C, Surmick D M and Witte M J 2014 *Spectrochim. Acta* B **99** 28
[9] Parigger C G, Woods A C, Surmick D M, Swafford L D and Witte M J 2014 *Spectrochim. Acta* B **99** 15
[10] Albert O, Roger S, Glinec Y, Loulergue J C, Etchepare J, Boulmer-Leborgne C, Perriére J and Millon E 2003 *Appl. Phys.* A **76** 319
[11] De Giacomo A 2003 *Spectrochim. Acta* B **58** 71
[12] Capitelli M 2004 *Spectrochim. Acta* B **59** 271
[13] Casavola A, Colonna G and Capitelli M 2003 *Appl. Surf. Sci.* **208** 85
[14] Griem H 1974 *Spectral Line Broadening by Plasma* (New York: Academic)
[15] De Giacomo A, Dell'Aglio M, Santagata A and Teghil R 2005 *Spectrochim. Acta* B **60** 935
[16] Parigger C G and Hornkohl J O 2011 *Spectrochim. Acta* A **81** 403
[17] Parigger C G, Woods A C, Keszler A, Nemes L, Hornkohl J O and Conf A I P 2012 *AIP Conf. Proc.* **1464** 628
[18] Hermann J, Perrone A and Dutouquet C 2001 *J. Phys.* B **34** 153
[19] Woods A C, Parigger C G and Hornkohl J O 2012 *Int. Rev. At. Mol. Phys.* **3** 103
[20] Aguilera J A and Aragón C 1861 *Spectrochim. Acta* A **59** 204
[21] Bogaerts A and Chen Z 2005 *Spectrochim. Acta* A **60** 1280

Chapter 28

[1] Hornkohl J O, Fleischmann J P, Surmick D M, Witte M J, Swafford L D, Woods A C and Parigger C G 2014 *J. Phys.: Conf. Ser.* 548 012040
[2] Parigger C G, Lewis J W L, Plemmons D P and Hornkohl J O 1996 Nitric oxide optical breakdown spectra and analysis by the use of the program NEQAIR *Laser Appl. Chem. Bio. Env. Anal.* **3** 85

[3] Hornkohl J O, Parigger C G and Lewis J W L 1991 *J. Quant. Spectrosc. Radiat. Transfer* **46** 405

[4] Parigger C G, Plemmons D H, Hornkohl J O and Lewis J W L 1994 *J. Quant. Spectrosc. Radiat. Transfer* **52** 707

[5] Parigger C G, Plemmons D H, Hornkohl J O and Lewis J W L 1995 *Appl. Opt.* **34** 3331

[6] Park C 1995 *Nonequilibrium Air Radiation (NEQAIR) Program: User's Manual* (Moffet Field, CA: NASA TM 86 707)

[7] Laoux C O 1993 Optical diagnostics and radiative emission of air plasmas *PhD Dissertation* Department of Mechanical Engineering, Stanford University, Stanford, CA

[8] Whiting E E 1995 Private communication

[9] Whiting E E, Park C, Liu Y, Arnold J O and Paterson J A 1996 *NEQAIR96, Nonequilibrium Radiative Transport and Spectra Program: User's Manual* (Moffet Field, CA 94 035: NASA TM 1389)

[10] Boulous M I, Fauchais P and Pfender E 1994 *Thermal Plasmas–Fundamentals and Applications* (New York: Plenum)

[11] Drakes J A, Pruitt D W, Howard R P and Hornkohl J O 1997 *J. Quant. Spectrosc. Radiat. Transfer* **57** 23

[12] Lewis J W L, Parigger C G, Hornkohl J O and Guan G 1999 Laser-induced optical breakdown plasma spectra and analyses with the program NEQAIR *37th Aerospace Sciences Meeting and Exhibit*

[13] Plemmons D H, Parigger C G, Lewis J W L and Hornkohl J O 1998 *Appl. Opt.* **37** 2493

[14] Ochkin V N 2009 *Spectroscopy of Low Temperature Plasma* (Weinheim: Wiley)

[15] Nemes L, Hornkohl J O and Parigger C G 2005 *Appl. Opt.* **44** 3686

[16] Parigger C G, Woods A C, Witte M J, Swafford L D and Surmick D M 2014 *J. Vis. Exp.* **84** 51250

[17] Nelder J A and Mead R 1965 *Comput. J.* **7** 308

[18] Lagarias J C, Reeds J A, Wright M H and Wright P E 1998 *SIAM J. Optim.* **9** 112

[19] Levin D A, Laux C O and Kruger C H 1999 *J. Quant. Spectrosc. Radiat. Transfer* **61** 377

[20] Hammack S D, Carter C D, Gord J R and Lee T 2012 *Appl. Opt.* **51** 8817

[21] Schultz C, Sick V, Heinze J and Stricker W 1997 *Appl. Opt.* **36** 3227

[22] Battles B E and Hanson R K 1995 *J. Quant. Spectrosc. Radiat. Transfer* **54** 521

[23] Harrington J E, Noble A R, Smith G P, Jeffries J B and Crosley D R 1995 Evidence for a new no production mechanism in flames paper # WSS/CI 95

[24] Rumminger M, Heberle N H, Dibble R W, Smith G P, Jeffries J B and Crosley D R 1995 Gas temperature above a porous radiant burner: comparison of measurements and model predictions paper # WSS/CI 95

[25] Labracherie L, Billiotte M and Houas L 1995 *J. Quant. Spectrosc. Radiat. Transfer* **54** 573

Chapter 29

[1] Miziolek A W, Palleschi V and Schechter I (ed) 2006 *Laser-Induced Breakdown Spectroscopy (LIBS)—Fundamentals and Applications* (New York: Cambridge University Press)

[2] Falcon R E 2012 *Cornell University Library, Astro-Ph* (Nash: Cornell University) http://arxiv.org/abs/1210.7197v1

[3] Falcon R E, Rochau G A, Bailey J E, Gomez T A, Montgomery M H, Winget D E and Nagayama T 2015 *Astrophys. J.* **806** 214

[4] Radon J 1917 *Ber. Sächs. Akad. Wissenschaft. Leipzig Math. Phys. Kl* **69** 262

[5] Radon J 1986 **5** 170
[6] Kunze H-J 2009 *Introduction to Plasma Spectroscopy* (Heidelberg: Springer)
[7] Cormack A M 1963 *J. Appl. Phys.* **34** 2722
[8] Cormack A M 1964 *J. Appl. Phys.* **35** 2908
[9] Deans S R 1983 *The radon transform and some of its applications*
[10] Merk S, Demidov A, Shelby D, Gornushkin I B, Panne U, Smith B W and Omenetto N 2013 *Appl. Spectrosc.* **67** 851
[11] Burger M, Skočić M and Bukvić S 2014 *Acta Part B.: At. Spectrosc.* **101** 51
[12] Pretzler G 1991 *Z. Naturforsch* **46a** 639
[13] Killer C 2014 Abel inversion algorithm http://www.mathworks.com/matlabcentral/fileexchange/43639-abel-inversion-algorithm
[14] Blades M W and Horlick G 1980 *Appl. Spectrosc.* **34** 696
[15] Blades M W 1983 *Appl. Spectrosc.* **37** 371
[16] Djurović S, Ćirišan M, Demura A V, Demchenko G V, Nikolić D, Gigosos M A and González M Á 2009 *Phys. Rev.* E **79** 046402
[17] Palomares J M, Torres J, Gigosos M A, van der Mullen J J A M, Gamero A and Sola A 2009 *Appl. Spectrosc.* **63** 1023
[18] Palomares J M, Torres J, Gigosos M A, van der Mullen J J A M, Gamero A and Sola A 2010 *J. Phys.: Conf. Ser.* **207** 012013
[19] Sobral H, Villagrán-Muniz M, Navarro-Gonzaález R and Raga A C 2000 *Appl. Phys. Lett.* **77** 3158
[20] Thiyagarajan M and Scharer J E 2008 *IEEE Trans. Plasma Sci.* **36** 2512
[21] Parigger C G, Gautam G and Surmick D M 2015 *Int. Rev. At. Mol. Phys.* **6** 43
[22] Arfken G B, Weber H J and Harris F E 2012 *Mathematical Methods for Physicists, A comprehensive Guide* seventh edition (New York: Academic)
[23] Oks E, Parigger C G and Plemmons D H 2003 *Appl. Opt.* **42** 5992
[24] Gautam G, Parigger C G, Surmick D M and Sherbini A M E L 2016 *J. Quant. Spect. Radiat. Transf.* **170** 189
[25] Parigger C G, Gautam G, Woods A C, Surmick D M and Hornkohl J O 2014 *Trends Appl. Spectrosc.* **11** 1
[26] Parigger C G, Woods A C, Surmick D M, Gautam G, Witte M J and Hornkohl J O 2015 *Spectrochim. Acta* B **107** 132
[27] Konjević N, Ivković M and Sakan N 2012 *Spectrochim. Acta* B **76** 16
[28] Ivković M, Konjević N and Pavlović Z 2015 *J. Quant. Spect. Radiat. Transf.* **154** 1
[29] Surmick D M and Parigger C G 2015 *Int. Rev. At. Mol. Phys.* **5** 71

Chapter 30

[1] Miziolek A W, Palleschi V and Schechter I (ed) 2006 *Laser-Induced Breakdown Spectroscopy (LIBS)—Fundamentals and Applications* (New York: Cambridge University Press)
[2] Singh J P and Thakur S N (ed) 2020 *Laser-Induced Breakdown Spectroscopy* (New York: Elsevier Science)
[3] Gautam G, Helstern C M, Drake K A and Parigger C G 2016 *Int. Rev. At. Mol. Phys.* **7** 45
[4] Gautam G and Parigger C G 2018 *Atoms* **6** 46
[5] Parigger C G, Helstern C M, Jordan B S, Surmick D M and Splinter R 2020 *Molecules* **25** 615

[6] Helstern C M 2020 Laser-induced breakdown spectroscopy and plasmas containing cyanide *PhD Dissertation* The University of Tennessee, Knoxville, Knoxville, TN
[7] Bethe H A, Fuchs K, Hirschfelder J O, Magee J L, Peierls R E and Neumann J 1947 *Blastwave*
[8] Taylor G I 1950 *Proc. Math. Phys. Eng. Sci.* **201** 159
[9] Sedov L I 1959 *Similarity and Dimensional Methods in Mechanics* (Cambridge, MA: Academic)
[10] Sedov L I 1946 *Prikl. Mat. Mech.* **10** 241
[11] Harith M A, Palleschi V, Salvetti A, Singh D P, Tropiano G and Vaselli M 1990 *Beams* **8** 247
[12] Parigger C G, Helstern C M and Gautam G 2019 *Atoms* **7** 74
[13] Parigger C G, Helstern C M and Gautam G 2017 *Int. Rev. At. Mol. Phys.* **8** 25
[14] Dackman M 2014 Laser-induced breakdown spectroscopy for analysis of high-density methane–oxygen mixtures *Master Thesis* The University of Tennessee, Knoxville, Knoxville, TN
[15] Griem H 1974 *Spectral Line Broadening by Plasma* (New York: Academic)
[16] Surmick D M 2016 Spectroscopic imaging of aluminum containing plasma *PhD Dissertation* The University of Tennessee, Knoxville, Knoxville, TN
[17] O'Haver T 2018 Peakfit algorithm https://www.mathworks.com/matlabcentral/fileexchange/23611-peakfit-m
[18] Parigger C G, Helstern C M and Gautam G 2020 *Symmetry* **12** 2116
[19] Parigger C G and Hornkohl J O 2020 *Quantum Mechanics of the Diatomic Molecule with Applications* (Bristol: IOP Publishing)
[20] Parigger C G, Woods A C, Surmick D M, Gautam G, Witte M J and Hornkohl J O 2015 *Spectrochim. Acta* B **107** 132
[21] Nelder J A and Mead R 1965 *Comput. J.* **7** 308
[22] Pretzler G and Naturforsch Z 1991 *Z. Naturforsch* **46a** 639
[23] Pretzler G, Jäger H, Neger T, Philipp H and Woisetschläger J 1992 *Z. Naturforsch.* A **47** 955
[24] Kandel Y P 2009 An experimental study of hydrogen balmer lines in pulsed laser plasma *PhD Dissertation* Wesleyan University, Middletown, CT
[25] Gornushkin I B, Shabanov S V and Panne U 2011 *J. Anal. At. Spectrom.* **26** 1457
[26] Killer C 2014 Abel inversion algorithm http://www.mathworks.com/matlabcentral/fileexchange/43639-abel-inversion-algorithm
[27] Parigger C G, Gautam G and Surmick D M 2015 *Int. Rev. At. Mol. Phys.* **6** 43
[28] Gautam G 2017 On laser-induced plasma containing hydrogen *PhD Dissertation* The University of Tennessee, Knoxville, Knoxville, TN
[29] Parigger C G, Surmick D M and Gautam G 2017 *J. Phys. Conf. Ser.* **810** 012012
[30] Gautam G, Parigger C G, Helstern C M and Drake K A 2017 *Appl. Opt.* **56** 9277
[31] Dardis J and Costello J T 2010 *Spectrochim. Acta* B **65** 535
[32] Zel'dovich Y B and Raizer Y P 1966 *Physics of Shock Waves and High-Temperature Hydrodynamic Phenomena* ed W D Hayes and R F Probstein Vol 1 (New York: Academic)

Appendix A

[1] Klein O 1929 *Zur Frage der Quantelung des asymmetrischen Kreisels* **58** 730
[2] Parigger C G and Hornkohl J O 2010 *Int. Rev. At. Mol. Phys.* **1** 25
[3] Hornkohl J O and Parigger C G 1996 *Am. J. Phys.* **64** 623

[4] Messiah A 1964 *Quantum Mechanics* (Amsterdam: North-Holland)
[5] Goldstein H, Poole C P and Safko J L 2001 *Classical Mechanics* 3rd edn (Reading, MA: Addison-Wesley)
[6] Davydov A S 1965 *Quantum Mechanics* (Oxford: Pergamon)
[7] Rose M E 1995 *Elementary Theory of Angular Momentum* (Mineola, NY: Dover)
[8] Brink D M and Satchler G R 1968 *Angular Momentum* (Oxford: Oxford University Press)
[9] Tinkham M 1964 *Group Theory and Quantum Mechanics* (New York: McGraw-Hill)
[10] Gottfried K 1989 *Quantum Mechanics* (Reading: Addison-Wesley)
[11] Baym G 1969 *Lectures on Quantum Mechanics* (London: Benjamin/Cummings)
[12] Shore B W and Menzel D H 1968 *Principles of Atomic Spectra* (Reading: Addison-Wesley)
[13] Judd B 1975 *Angular Momentum Theory for Diatomic Molecules* (New York: Academic)
[14] Mizushima M 1975 *The Theory of Rotating Diatomic Molecules* (New York: Wiley)
[15] Van Vleck J H 1951 The coupling of angular momentum vectors in molecules *Rev. Mod. Phys.* **23** 213
[16] Freed K F 1966 *J. Chem. Phys.* **45** 4214
[17] Kovács I 1969 *Rotational Structure in the Spectra of Diatomic Molecules* (New York: American Elsevier)
[18] Hougen J T 2001 *The Calculation of Rotational Energy Levels and Rotational Line Intensities in Diatomic Molecules* (Gaithersburg, MD: National Institute of Standards and Technology) http://physics.nist.gov/DiatomicCalculations. Originally published as *The Calculation of Rotational Energy Levels and Rotational Line Intensities in Diatomic Molecules*, J. T. Hougen, NBS Monograph 115 (1970)
[19] Miller T A, Carrington A and Levy D H 1970 *Adv. Chem. Phys.* **18** 149
[20] Brown J M and Carrington A 2003 *Rotational Spectroscopy of Diatomic Molecules* (Cambridge: Cambridge University Press)
[21] Lefebvre-Brion H and Field R W 2004 *The Spectra and Dynamics of Diatomic Molecules* (New York: Elsevier/Academic)
[22] Bunker P R and Jensen P 1998 *Molecular Symmetry and Spectroscopy* 2nd edn (Ottawa: NRC))

Appendix B

[1] Parigger C G and Hornkohl J O 2010 *Int. Rev. At. Mol. Phys.* **1** 25
[2] Van Vleck J H 1951 The coupling of angular momentum vectors in molecules *Rev. Mod. Phys.* **23** 213
[3] Judd B 1975 *Angular Momentum Theory for Diatomic Molecules* (New York: Academic)
[4] Mizushima M 1975 *The Theory of Rotating Diatomic Molecules* (New York: Wiley)
[5] Freed K F 1966 *J. Chem. Phys.* **45** 4214
[6] Kovács I 1969 *Rotational Structure in the Spectra of Diatomic Molecules* (New York: American Elsevier)
[7] Hougen J T 2001 *The Calculation of Rotational Energy Levels and Rotational Line Intensities in Diatomic Molecules* (Gaithersburg, MD: National Institute of Standards and Technology) http://physics.nist.gov/DiatomicCalculations. Originally published as *The Calculation of Rotational Energy Levels and Rotational Line Intensities in Diatomic Molecules*, J. T. Hougen, NBS Monograph 115 (1970)
[8] Miller T A, Carrington A and Levy D H 1970 *Adv. Chem. Phys.* **18** 149
[9] Zare R N, Schmeltekopf A L, Harrop W J and Albritton D L 1973 *J. Mol. Spectrosc.* **46** 37
[10] Brown J M and Howard B J 1976 *Mol. Phys.* **31** 1517

[11] Lefebvre-Brion H and Field R W 2004 *The Spectra and Dynamics of Diatomic Molecules* (New York: Elsevier/Academic)
[12] Gottfried K 1989 *Quantum Mechanics* (Reading: Addison-Wesley)

Appendix C

[1] Wiese W L 1991 *Spectrochim. Acta* B **46** 831
[2] Hornkohl J O, Parigger C G and Lewis J W L 1991 *J. Quant. Spectrosc. Radiat. Transfer* **46** 405

Appendix D

[1] Guelachvili G, Amiot C and Bacis R 1978 *Can. J. Phys.* **56** 251
[2] Macki A G and Wells J S 1991 *Wavenumber Calibration tables from Heterodyne Frequency Measurements* NIST Special Publication 821 (Washington, DC: NIST)
[3] Zare R N, Schmeltekopf A L, Harrop W J and Albritton D L 1973 *J. Mol. Spectrosc.* **46** 37
[4] Engleman R Jr+, Rouse P E, Peek H M and Baiamonte V D 1970 *Eta and Gamma Band Systems of Nitric Oxide* Los Alamos Sci. Lab. Report LA-4364, Los Alamos, NM
[5] Hornkohl J O and Parigger C G 1996 *Am. J. Phys.* **64** 623
[6] Lefebvre-Brion H and Field R W 2004 *The Spectra and Dynamics of Diatomic Molecules* (New York: Elsevier/Academic)
[7] Thompson W J 1994 *Angular Momentum* (New York: Wiley)

Appendix E

[1] Hornkohl J O and Parigger C G 2017 *Int. J. Mol. Theor. Phys.* **1** 00103
[2] Zare R N, Schmeltekopf A L, Harrop W J and Albritton D L 1973 *J. Mol. Spectrosc.* **46** 37
[3] Brown J M, Hougen J T, Huber K P, Johns J W C, Kopp I, Lefebvre-Brion H, Merer A J, Ramsay D A, Rostas J and Zare R N 1975 *J. Mol. Spectrosc.* **55** 500
[4] Hougen J T 2021 *The Calculation of Rotational Energy Levels and Rotational Line Intensities in Diatomic Molecules* (Gaithersburg, MD: National Institute of Standards and Technology) http://physics.nist.gov/DiatomicCalculations, 2001. Originally published as *The Calculation of Rotational Energy Levels and Rotational Line Intensities in Diatomic Molecules*, J. T. Hougen, NBS Monograph 115 (1970)
[5] Røeggen I 1971 *Theor. Chim. Acta* **21** 398
[6] Judd B 1975 *Angular Momentum Theory for Diatomic Molecules* (New York: Academic)
[7] Larsson M 1981 *Phys. Scr.* **23** 835
[8] Wigner E and Witmer E E 1928 *Z. Phys.* **51** 859 H. Hettema, *Quantum Chemistry: Classic Scientific Papers*, p. 287, (Singapore: World Scientific) 2000
[9] Condon E U and Shortley G 1953 *The Theory of Atomic Spectra* (Cambridge: Cambridge University Press)
[10] Faris G W and Cosby P C 1992 *J. Chem. Phys.* **97** 7073
[11] Parigger C G, Woods A C, Surmick D M, Gautam G, Witte M J and Hornkohl J O 2015 *Spectrochim. Acta* B **107** 132

Appendix F

[1] Hornkohl J O and Parigger C G 2017 *Int. J. Mol. Theor. Phys.* **1** 00102
[2] Ram R S, Davis S P, Wallace L, Englman R, Appadoo D R T and Bernath P F 2006 *J. Mol. Spectrosc.* **237** 225

[3] Brooke J S A, Ram R S, Western C M, Li G, Schwenke D W and Bernath P F 2014 *J. Quant. Spectrosc. Radiat. Transfer* **210** Astrophys. J. Supp. Series
[4] Ito H, Fukuda Y, Ozaki Y, Kondow T and Kuchitsu K 1987 *J. Mol. Spectrosc.* **121** 84
[5] Western C M 2017 *J. Quant. Spectrosc. Radiat. Transfer* **186** 221
[6] Engleman R 1974 *J. Mol. Spectrosc.* **49** 106
[7] Kroto H W 2016 National Solar Observatory (NSO) at Kitt Peak, McMath-Pierce Fourier Transform Spectrometer (FTS) data, (accessed December 20, 2016). ftp://vso.nso.edu/FTS_cdrom/FTS30/920212R0.005.
[8] Parigger C G, Woods A C, Surmick D M, Gautam G, Witte M J and Hornkohl J O 2015 *Spectrochim. Acta* B **107** 132
[9] Yurchenko S N, Lodi L, Tennyson J and Stolyarov A V 2016 *Comput. Phys. Commun.* **202** 262
[10] Wigner E and Witmer E E 1928 *Z. Phys.* **51** 859
Hettema H 2000 *Quantum Chemistry: Classic Scientific Papers* p 287 (Singapore: World Scientific)
[11] Zare R N, Schmeltekopf A L, Harrop W J and Albritton D L 1973 *J. Mol. Spectrosc.* **46** 37
[12] Howard B J and Brown J M 1976 *J. Mol. Phys.* **31** 1517
[13] Lefebvre-Brion H and Field R W 2004 *The Spectra and Dynamics of Diatomic Molecules* (New York: Elsevier/Academic)
[14] Brown J M and Carrington A 2003 *Rotational Spectroscopy of Diatomic Molecules* (Cambridge: Cambridge University Press)
[15] Condon E U and Shortley G 1953 *The Theory of Atomic Spectra* (Cambridge: Cambridge University Press)
[16] Hilborn R C 1982 *Am. J. Phys.* **50** 982 http://arxiv.org/ftp/physics/papers/0202/0202029.pdf
[17] Thorne A P 1988 *Spectrophysics* 2nd edn (London: Chapman and Hall)
[18] Rothman L S *et al* 1998 *J. Quant. Spectrosc. Radiat. Transfer* **60** 665
[19] Brown J M, Hougen J T, Huber K P, Johns J W C, Kopp I, Lefebvre-Brion H, Merer A J, Ramsay D A, Rostas J and Zare R N 1975 *J. Mol. Spectrosc.* **55** 500
[20] Kovács I 1969 Rotational Structure in the Spectra of Diatomic Molecules *Rotational Structure in the Spectra of Diatomic Molecules* (American Elsevier: New York)
[21] Li G, Harrison J J, Ram R S, Western C M and Bernath P F 2012 *J. Quant. Spectrosc. Radiat. Transfer* **113** 67

Appendix G

[1] Amiot C 1983 *Astrophys. J. Suppl. Ser.* **52** 329
[2] Roux F, Michaud F and Vervloet M 1989 *Can. J. Phys.* **67** 143
[3] Lazdinis S S and Carpenter R F 1973 *J. Chem. Phys.* **59** 5203
[4] Michaud F, Roux F, Davis S P, Nguyen A-D and Laux C O 2000 *J. Mol. Spectrosc.* **203** 1

Appendix H

[1] Hornkohl J O and Woods A C 2014 *J. Phys.: Conf. Ser.* 548 012033
[2] Singh J P and Thakur S N (ed) 2020 *Laser-Induced Breakdown Spectroscopy* (New York: Elsevier Science)
[3] Musazzi S and Perini U (ed) 2014 *Laser-Induced Breakdown Spectroscopy* (Heidelberg: Springer)

[4] Cremers D E and Radziemski L J 2006 *Handbook of Laser-Induced Breakdown Spectroscopy* (New York: Wiley)

[5] Noll R 2011 *Laser-Induced Breakdown Spectroscopy.* (Heidelberg: Springer)

[6] Singh J P and Thakur S N (ed) 2007 *Laser-Induced Breakdown Spectroscopy* (Amsterdam: Elsevier Science)

[7] Miziolek A W and Palleschi V (ed) 2006 *Laser-Induced Breakdown Spectroscopy (LIBS)—Fundamentals and Applications* (New York: Cambridge University Press)

[8] Parigger C G 2006 Laser-induced breakdown in gases: Experiments and simulation *Laser-Induced Breakdown Spectroscopy (LIBS)—Fundamentals and Applications* ed A W Miziolek, V Palleschi and I Schechter (New York: Cambridge University Press)

[9] Parigger C G, Surmick D M, Helstern C M, Gautam G, Bol'shakov A A and Russo R 2020 Molecular laser-induced breakdown spectrosocpy *Laser-Induced Breakdown Spectroscopy* ed J P Singh and S N Thakur (New York: Elsevier Science) ch 7

[10] Merten J, Jones M, Hoke S and Allen S A 2014 *J. Phys.: Conf. Ser.* 548 012042

[11] Parigger C G, Helstern C M and Gautam G 2019 *Atoms* **7** 7030074

[12] Tiwari P K, Rai N K, Kumar R, Parigger C G and Rai A K 2019 *Atoms* **7** 7030071

[13] Surmick D M, Dagel D J and Parigger C G 2019 *Atoms* **7** accepted

[14] Parigger C G, Sherbini A M E L and Splinter R 2019 *J. Phys.: Conf. Ser.* accepted

[15] Wigner E and Witmer E E 1928 *Z. Phys.* **51** 859
Hettema H 2000 *Quantum Chemistry: Classic Scientific Papers* p 287 (Singapore: World Scientific)

[16] Born M and Oppenheimer R 1927 *Ann. Phys.* **84** 457
Hettema H 2000 *Quantum Chemistry: Classic Scientific Papers* p 1 (Singapore: World Scientific)

[17] Nemes L, Keszler A M, Hornkohl J O and Parigger C G 2005 *Appl. Opt.* **44** 3661

[18] Nemes L, Hornkohl J O and Parigger C G 2005 *Appl. Opt.* **44** 3686

[19] Rose M E 1995 *Elementary Theory of Angular Momentum* (Mineola, NY: Dover)

[20] Edmonds A R 1974 *Angular Momentum in Quantum Mechanics* 2nd edn (Princeton, NJ: Princeton University Press)

[21] Brink D M and Satchler G R 1993 *Angular Momentum* 3rd edn (Oxford: Oxford University Press)

[22] Biedenharn L C and Louck J D 2009 *Angular Momentum in Quantum Physics* (Cambridge: Cambridge University Press)

[23] Zare R N 1988 *Angular Momentum* (New York: Wiley)

[24] Thompson W J 1994 *Angular Momentum* (New York: Wiley)

[25] Varshalovich D A, Moskalev A N and Khersonskii V K 1988 *Quantum Theory of Angular Momentum* (Singapore: World Scientific)

[26] Kovács I 1969 *Rotational Structure in the Spectra of Diatomic Molecules* (New York: American Elsevier)

[27] Lefebvre-Brion H and Field R W 2004 *The Spectra and Dynamics of Diatomic Molecules* (New York: Elsevier/Academic)

[28] Brown J M and Carrington A 2003 *Rotational Spectroscopy of Diatomic Molecules* (Cambridge: Cambridge University Press)

[29] Zare R N, Schmeltekopf A L, Harrop W J and Albritton D L 1973 *J. Mol. Spectrosc.* **46** 37

[30] Hornkohl J O, Nemes L and Parigger C G 2009 Spectroscopy, dynamics and molecular theory of carbon plasmas and vapors *Advances in the Understanding of the Most Complex High-Temperature Elemental System* ed L Nemes and S Irle (Singapore: World Scientific) ch 4

[31] Huang K and Born M 1954 *Dynamical Theory of Crystal Lattices* (Oxford: Clarendon)

Appendix I

[1] Parigger C G, Woods A C, Keszler A, Nemes L and Hornkohl J O 2012 *AIP Conf. Proc.* **1464** 628

Appendix J

[1] Parigger C G, Woods A C, Surmick D M, Gautam G, Witte M J and Hornkohl J O 2015 *Spectrochim. Acta* B **107** 132
[2] *MATLAB Release R2022a Update 5* (MA: Natick)
[3] Parigger C G and Hornkohl J O 2020 *Quantum Mechanics of the Diatomic Molecule with Applications* (Bristol: IOP Publishing)
[4] Corney A 1977 *Atomic and Laser Spectroscopy* (Oxford: Clarendon)
[5] Parigger C G 2022 *Foundations* **2** 934
[6] Parigger C G 2023 *Foundations* **3** 1

Appendix K

[1] Pretzler G and Naturforsch Z 1991 *Z. Naturforsch* **46a** 639
[2] Arfken G B, Weber H J and Harris F E 2012 *Mathematical Methods for Physicists, A Comprehensive Guide* 7th edn (New York: Academic)
[3] Pretzler G, Jäger H, Neger T, Philipp H and Woisetschläger J 1992 *Z. Naturforsch.* A **47** 955
[4] Killer C 2014 http://www.mathworks.com/matlabcentral/fileexchange/43639-abel-inversion-algorithm.
[5] *MATLAB Release R2022a Update 5* (MA: Natick)
[6] Helstern C M 2020 Laser-induced breakdown spectroscopy and plasmas containing cyanide *PhD Dissertation* (University of Tennessee)

Appendix L

[1] Ioannidis J P A 2023 *October 2023 data-update for: Updated science-wide author databases of standardized citation indicators,* Elsevier Data Repository, Electronic data https://ecebm.com/2023/10/04/stanford-university-names-worlds-top-2-scientists-2023/
[2] Parigger C G 2023 *Int. Rev. At. Mol. Phys.* **14** 89
[3] Parigger C G, Drake K A, Helstern C M and Gautam G 2018 *Atoms* **6** 36
[4] Parigger C G 2020 *Contrib. Astronom. Observat. Skalnaté Pleso* **50** 1
[5] Parigger C G, Helstern C M, Gautam G and Drake D A 2019 *J. Phys.: Conf. Ser.* 1289 012001
[6] Parigger C G, Helstern C M and Gautam G 2019 *Atoms* **7** 63
[7] Surmick D M and Parigger C G 2019 *Atoms* **7** 101
[8] Parigger C G, Sherbini A M E L and Splinter R 2019 *J. Phys.: Conf. Ser.* 1253 012001
[9] Gautam G and Parigger C G 2018 *Atoms* **6** 46
[10] Parigger C G 2019 *Atoms* **7** 61
[11] Parigger C G, Helstern C M and Gautam G 2020 *Symmetry* **12** 2116
[12] Parigger C G, Helstern C M and Gautam G 2019 *Atoms* **7** 74
[13] Helstern C M and Parigger C G 2019 *J. Phys.: Conf. Ser.* 1289 012016
[14] Parigger C G and Helstern C M 2023 *J. Phys.: Conf. Ser.* 2439 012003
[15] Surmick D M, Dagel D J and Parigger C G 2019 *Atoms* **7** 86

[16] Parigger C G, Helstern C M, Jordan B S, Surmick D M and Splinter R 2020 *Molecules* **25** 615
[17] Parigger C G 2020 *Spectrochim. Acta* B **179** 106122
[18] Parigger C G 2021 *Foundations* **1** 208
[19] Parigger C G 2023 *Foundations* **3** 1
[20] Parigger C G 2022 *Foundations* **2** 934
[21] Parigger C G 2023 *Atoms* **11** 62
[22] Parigger C G 2023 *Preprints* **2023** 2023050423
[23] Parigger C G 2023 *Preprints* **2023** 2023041258
[24] Parigger C G, Helstern C M, Jordan B S, Surmick D M and Splinter R 2020 *Molecules* **25** 988
[25] Parigger C G and Helstern C M 2023 *J. Phys.: Conf. Ser.* 2439 012004
[26] Rai A K, Pati J K, Parigger C G, Dubey S, Rai A K, Bhagabaty B, Mazumdar A C and Duorah K 2020 *Molecules* **25** 984
[27] Rai A K, Pati J K, Parigger C G and Rai A K 2019 *Atoms* **7** 72
[28] Pathak A K, Rai N K, Kumar R, Rai P K, Rai A K and Parigger C G 2018 *Atoms* **6** 42
[29] Kumar T, Rai P K, Rai A K, Rai N K, Rai A K, Parigger C G, Watal G and Yadav S 2022 *Foundations* **2** 981
[30] Sherbini A M E L, Sherbini A E E L and Parigger C G 2018 *Atoms* **6** 44
[31] Sherbini1 A M E L, Sherbini A E E L, Parigger C G and Sherbini T M E L 2019 *J. Phys.: Conf. Ser.* 1289 012002
[32] Sherbini A M E L, Farash A H E L, Sherbini T M E L and Parigger C G 2019 *Atoms* **7** 73
[33] Nemes L and Parigger C G 2023 *Foundations* **3** 16
[34] Parigger C G, Surmick D M, Helstern C M, Gautam G, Bol'shakov A A and Russo R 2020 Molecular laser-induced breakdown spectroscopy *Laser Induced Breakdown Spectroscopy* ed J P Singh and S N Thakur 2nd edn (New York: Elsevier)
[35] Parigger C G and Hornkohl J O 2020 *Quantum Mechanics of the Diatomic Molecule with Applications* (Bristol: IOP Publishing)
[36] McKemmish L K 2021 *WIREs Comput. Mol. Sci.* **11** e1520
[37] Tennyson J *et al* 2020 *J. Quant. Spectrosc. Radiat. Transf.* **255** 107228