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## **Publication List**

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- 1 J.E. Plamondon, R.J. Buenker, D.J. Koopman and R.J. Dolter, **The Dipole Moment of Styrene**, *Proc. Iowa Acad. Sci.* **70**, 163-166 (1963).
- 2 R.J. Buenker and G.N. Schulte, **Application of Guggenheim's Short Formula to the Calculation of Dipole Moments**, *Proc. Iowa Acad. Sci.* **70**, 187-190 (1963).
- 3 R.F. Robertson and R.J. Buenker, **Elastic Moduli of Bisphenol A Polycarbonate**, *J. Poly. Sci.* **2**, 4889-4901 (1964).
- 4 K.W. Kraus, G.N. Schulte, R.J. Dolter, R.J. Buenker, J.E. Plamondon and D.J. Koopman, **The Dipole Moments and Molar Refractions of Several Trans-Beta-Nitrostyrenes**, *Proc. Iowa Acad. Sci.* **71**, 208-211 (1964).
- 5 S.D. Peyerimhoff, R.J. Buenker and L.C. Allen, **Geometry of Molecules. I. Wavefunctions for Some Six- and Eight-Electron Polyhydrides**, *J. Chem. Phys.* **45**, 734-749 (1966).
- 6 R.J. Buenker, S.D. Peyerimhoff, L.C. Allen and J.L. Whitten, **Geometry of Molecules. II. Diborane and Ethane**, *J. Chem. Phys.* **45**, 2835-2847 (1966).
- 7 R.J. Buenker and S.D. Peyerimhoff, **Geometry of Molecules. III. F<sub>2</sub>O, Li<sub>2</sub>O, FOH, LiOH**, *J. Chem. Phys.* **45**, 3682-3700 (1966).
- 8 S.D. Peyerimhoff, R.J. Buenker and J.L. Whitten, **Study of Linear Stretch in Polyatomic Molecules: Accurate SCF MO Wavefunctions for CO<sub>2</sub> and BeF<sub>2</sub>**, *J. Chem. Phys.* **46**, 1707-1716 (1967).
- 9 R.J. Buenker, S.D. Peyerimhoff and J.L. Whitten, **Theoretical Analysis of the Effects of Hydrogenation in Hydrocarbons: Accurate SCF MO Wavefunctions for C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>4</sub>, and C<sub>2</sub>H<sub>6</sub>**, *J. Chem. Phys.* **46**, 2029-2039 (1967).
- 10 S.D. Peyerimhoff and R.J. Buenker, **Geometry of Ozone and Azide Ion in Ground and Certain Excited States**, *J. Chem. Phys.* **47**, 1953-1966 (1967).
- 11 S.D. Peyerimhoff and R.J. Buenker, **Ab Initio Study of the Molecular Geometry and Properties of Nitrosyl Fluoride**, *Theor. Chim. Acta* **9**, 103-115 (1967).
- 12 R.J. Buenker and S.D. Peyerimhoff, **Ab Initio Study on the Stability and Geometry of Cyclobutadiene**, *J. Chem. Phys.* **48**, 354-373 (1968).
- 13 R.J. Buenker, **Theoretical Study of the Rotational Barriers of Allene, Ethylene, and Related Systems**, *J. Chem. Phys.* **48**, 1368-1379 (1968).
- 14 S.D. Peyerimhoff and R.J. Buenker, **Further Study of Umbrella vs Bridged Geometries: SCF-MO and CI Calculations for C<sub>2</sub>H<sub>6</sub><sup>++</sup> and Ammonia Borane**, *J. Chem. Phys.* **49**, 312-325 (1968).

- 15 R.J. Buenker, J.L. Whitten and J.D. Petke, ***Ab Initio* SCF MO and CI Calculations on the Electronic Spectrum of Benzene**, *J. Chem. Phys.* **49**, 2261-2267 (1968).
- 16 S.D. Peyerimhoff and R.J. Buenker, **Theoretical Study of the Geometry and Spectrum of Nitrous Oxide**, *J. Chem. Phys.* **49**, 2473-2487 (1968).
- 17 R.J. Buenker and S.D. Peyerimhoff, **CI Method for the Study of General Molecular Potentials**, *Theor. Chim. Acta* **12**, 183-199 (1968).
- 18 R.J. Buenker and J.L. Whitten, ***Ab Initio* SCF MO and CI Studies of the Electronic States of Butadiene**, *J. Chem. Phys.* **49**, 5381-5387 (1968).
- 19 S.D. Peyerimhoff and R.J. Buenker, **Theoretical Comparison of Formic Acid and the Formate Ion**, *J. Chem. Phys.* **50**, 1846-1861 (1969).
- 20 R.J. Buenker and S.D. Peyerimhoff, ***Ab Initio* SCF Calculations for Azulene and Naphthalene**, *Chem. Phys. Letters* **3**, 37-42 (1969).
- 21 R.J. Buenker and S.D. Peyerimhoff, **Theoretical Study of the Geometry, Reactivity, and Spectrum of Cyclopropane**, *J. Phys. Chem.* **73**, 1299-1313 (1969).
- 22 R.J. Buenker and S.D. Peyerimhoff, **Theoretical Comparison of Tetrahedrane and Cyclobutadiene by *Ab Initio* Techniques**, *J. Am. Chem. Soc.* **91**, 4342-4346 (1969).
- 23 S.D. Peyerimhoff and R.J. Buenker, **Theoretical Study of Cyclopropene and its C<sub>3</sub>H<sub>4</sub> Isomers**, *Theor. Chim. Acta* **14**, 305-318 (1969).
- 24 S.D. Peyerimhoff and R.J. Buenker, **Study of the Geometry and Spectra of the Allylic Systems by *Ab Initio* Methods**, *J. Chem. Phys.* **51**, 2528-2537 (1969).
- 25 R.J. Buenker and S.D. Peyerimhoff, **Combined SCF and CI Method for the Calculation of Electronically Excited States of Molecules: Potential Curves for the Low-lying States of Formaldehyde**, *J. Chem. Phys.* **53**, 1368-1384 (1970).
- 26 K.W. Kraus, R.J. Buenker, R.J. Dolter, G.E. Petrowski, R.T. Bogan, J.E. Plamondon, J.J. Miller, D.L. Whalen and D.J. Koopman, **The Dipole Moments, Molar Refractions and Ultraviolet Spectra of Several Substituted Alkylnitrostyrenes**, *Proc. Iowa Acad. Sci.* **76**, 127-134 (1969).
- 27 S.K. Shih, R.J. Buenker, S.D. Peyerimhoff and B. Wirsam, **Comparison of Cartesian and Lobe Function Gaussian Basis Sets**, *Theor. Chim. Acta* **18**, 277-289 (1970).
- 28 S.D. Peyerimhoff and R.J. Buenker, **Comparison of the Molecular Structure and Spectra of Benzene and Borazine**, *Theor. Chim. Acta* **19**, 1-19 (1970).

- 29 S.D. Peyerimhoff, R.J. Buenker, W.E. Kammer and H. Hsu, **Calculation of the Electronic Spectrum of Formaldehyde**, *Chem. Phys. Letters* **8**, 129-135 (1971).
- 30 K. Hsu, R.J. Buenker and S.D. Peyerimhoff, **Theoretical Determination of the Reaction Path in the Prototype Electrocyclic Transformation between Cyclobutene and *cis*-Butadiene. Thermochemical Process**, *J. Am. Chem. Soc.* **93**, 2117-2127 (1971).
- 31 R.J. Buenker, S.D. Peyerimhoff and W.E. Kammer, **Combined SCF and CI Calculations for the Low-lying Rydberg and Valence Excited States of Ethylene**, *J. Chem. Phys.* **55**, 814-827 (1971).
- 32 R.J. Buenker, S.D. Peyerimhoff and K. Hsu, **Analysis of Qualitative Theories for Electrocyclic Transformations Based on the Results of *Ab Initio* Self-Consistent-Field and Configuration-Interaction Calculations**, *J. Am. Chem. Soc.* **93**, 5005-5013 (1971).
- 33 R.J. Buenker, S.D. Peyerimhoff and H.L. Hsu, **A New Interpretation for the Structure of the V-N Bands of Ethylene**, *Chem. Phys. Letters* **11**, 65-70 (1971).
- 34 R.J. Buenker and S.D. Peyerimhoff, **Extension of Walsh's Rules to More General Systems**, *Theor. Chim. Acta* **24**, 132-146 (1972).
- 35 K. Hsu, R.J. Buenker and S.D. Peyerimhoff, **The Role of Ring Torsion in the Electrocyclic Transformation between Cyclobutene and Butadiene. A Theoretical Study**, *J. Am. Chem. Soc.* **94**, 5639-5644 (1972).
- 36 S.K. Shih, R.J. Buenker, S.D. Peyerimhoff and C.J. Michejda, **Nonempirical Calculations of the Reaction Surface for the Addition of the Amino Radical to Ethylene**, *J. Am. Chem. Soc.* **94**, 7620-7627 (1972).
- 37 P. Merlet, S.D. Peyerimhoff and R.J. Buenker, ***Ab Initio* Study of the Hydrogen Bond in  $[\text{H}_3\text{N}-\text{H}\cdots\text{H}_3]^+$** , *J. Am. Chem. Soc.* **94**, 8301-8308 (1972).
- 38 S.D. Peyerimhoff and R.J. Buenker, **Comparison of Various CI Treatments for the Description of Potential Curves for the Lowest Three States of  $\text{O}_2$** , *Chem. Phys. Letters* **16**, 235-243 (1972).
- 39 S.K. Shih, R.J. Buenker and S.D. Peyerimhoff, **Non-empirical Calculations on the Electronic Spectrum of Butadiene**, *Chem. Phys. Letters* **16**, 244-251 (1972).
- 40 S.D. Peyerimhoff and R.J. Buenker, **Vibrational Analysis of the Electronic Spectrum of Ethylene Based on *Ab Initio* SCF-CI Calculations**, *Theor. Chim. Acta* **27**, 243-264 (1972).
- 41 R.J. Buenker and S.D. Peyerimhoff, **Molecular Geometry and the Mulliken-Walsh Molecular Orbital Model. An *Ab Initio* Study**, *Chem. Rev.* **74**, 127-188 (1974).

- 42 R.J.Buenker, **SCF and CI Calculations of Bimolecular Reaction Surfaces**, in: *Chemical and Biochemical Reactivity* (The Jerusalem Symposia on Quantum Chemistry and Biochemistry, VI), edited by E.D. Bergmann and B. Pullman (Israel Academy of Sciences and Humanities, Jerusalem, 1974). pp. 157-165.
- 43 S.D. Peyerimhoff and R.J. Buenker, **Ab Initio Calculations for Excited States of Molecules**, in: *Chemical Spectroscopy and Photochemistry in the Vacuum Ultraviolet* (NATO ASI Series C8), edited by C. Sandorfy, P.J. Ausloos and M.B. Robin (Reidel, Dordrecht, 1974), pp. 257-286.
- 44 S.D. Peyerimhoff and R.J. Buenker, **Ab Initio Calculations for Reaction Surfaces Involving Free Radicals**, *Ber. Bunsenges. Phys. Chem.* **78**, 119-127 (1974).
- 45 P.J. Bruna, S.D. Peyerimhoff, R.J. Buenker and P. Rosmus, **Non-empirical SCF and CI Study of the Ground and Excited States of Thioformaldehyde**, *Chem. Phys.* **3**, 35-53 (1974).
- 46 P. Merlet, S.D. Peyerimhoff, R.J. Buenker and S.K. Shih, **Ab Initio SCF and CI Study of the Electrocyclic Transformations of Cyclopropyl and Allyl Systems**, *J. Am. Chem. Soc.* **96**, 959-969 (1974).
- 47 R.J. Buenker and S.D. Peyerimhoff, **Individualized Configuration Selection in CI Calculations with Subsequent Energy Extrapolation**, *Theor. Chim. Acta* **35**, 33-58 (1974).
- 48 K. Vasudevan, S.D. Peyerimhoff and R.J. Buenker, **Ab Initio Study of the  $\text{HN}_2^+$  Molecule Ion and its Dissociation Products in Ground and Excited States**, *Chem. Phys.* **5**, 149-165 (1974).
- 49 U. Fischbach, R.J. Buenker and S.D. Peyerimhoff, **Non-empirical Calculations on the Rydberg States of Ethylene**, *Chem. Phys.* **5**, 265-276 (1974).
- 50 S.K. Shih, R.J. Buenker and S.D. Peyerimhoff, **Theoretical Investigation of the Cyclic Conformer of Ozone**, *Chem. Phys. Letters* **28**, 463-470 (1974).
- 51 R.J. Buenker and S.D. Peyerimhoff, **Calculations on the Electronic Spectrum of Water**, *Chem. Phys. Letters* **29**, 253-259 (1974).
- 52 S.D. Peyerimhoff and R.J. Buenker, **A Series of Electronic Spectral Calculations Using Nonempirical CI Techniques**, in: *Advances in Quantum Chemistry*, Vol. 9, edited by P.O. Löwdin (Academic Press, New York, 1975), pp. 69-104.
- 53 K. Vasudevan, S.D. Peyerimhoff, R.J. Buenker, W.E. Kammer and H.L. Hsu, **Theoretical Study of the Electronic Spectrum of Diimide by Ab Initio Methods**, *Chem. Phys.* **7**, 187-209 (1975).

- 54 R.J. Buenker and S.D. Peyerimhoff, ***Ab Initio* Calculations on the Electronic Spectrum of Ethane**, *Chem. Phys.* **8**, 56-67 (1975).
- 55 K. Vasudevan, S.D. Peyerimhoff and R.J. Buenker, ***Ab Initio* SCF and CI Study of the Ground and Excited States of the HN<sub>2</sub> Radical**, *J. Mol. Struct.* **29**, 285-297 (1975).
- 56 R.J. Buenker and S.D. Peyerimhoff, **Theoretical Study of the Vertical Electronic Spectrum of O<sub>2</sub>: Mixing of Valence and Rydberg States**, *Chem. Phys.* **8**, 324-337 (1975).
- 57 R.J. Buenker and S.D. Peyerimhoff, **All-Valence-Electron Configuration Mixing Calculations for the Characterization of the  ${}^1(\pi,\pi^*)$  States of Ethylene**, *Chem. Phys.* **9**, 75-89 (1975).
- 58 R.J. Buenker and S.D. Peyerimhoff, ***Ab Initio* Study of the Mixing of Valence and Rydberg States in O<sub>2</sub>: CI Potential Curves for the  ${}^3\Sigma_u^-$ ,  ${}^3\Delta_u$  and  ${}^3\Pi_u$  States**, *Chem. Phys. Letters* **34**, 225-231 (1975).
- 59 R.J. Buenker and S.D. Peyerimhoff, **Energy Extrapolation in CI Calculations**, *Theor. Chim. Acta* **39**, 217-228 (1975).
- 60 P.J. Bruna, S.D. Peyerimhoff and R.J. Buenker, ***Ab Initio* Investigation of the HCO<sup>+</sup> and COH<sup>+</sup> Molecule-Ions: Structure and Potential Surfaces for Dissociation in Ground and Excited States**, *Chem. Phys.* **10**, 323-334 (1975).
- 61 A.A. Wu, S.D. Peyerimhoff and R.J. Buenker, **Theoretical Study of the Electronic Spectrum of HNO Using SCF and CI Calculations**, *Chem. Phys. Letters* **35**, 316-322 (1975).
- 62 S.T. Elbert, S.D. Peyerimhoff and R.J. Buenker, **All-Valence-Electron CI Calculations on the Electronic Spectrum of Diborane**, *Chem. Phys.* **11**, 25-40 (1975).
- 63 R.J. Buenker and S.D. Peyerimhoff, **Mixed Valence-Rydberg States**, *Chem. Phys. Letters* **36**, 415-422 (1975).
- 64 P.J. Bruna, R.J. Buenker and S.D. Peyerimhoff, ***Ab Initio* Study of the Structure, Isomers and Vertical Electronic Spectrum of the Formyl Radical HCO**, *J. Mol. Struct.* **32**, 217-233 (1976).
- 65 R.J. Buenker and S.D. Peyerimhoff, **All-Valence-Electron CI Study of the Ground and Lowest Excited States of the Hydroperoxyl Radical**, *Chem. Phys. Letters* **37**, 208-211 (1976).
- 66 W.H.E. Schwarz and R.J. Buenker, **Use of the Z+1-Core Analogy Model: Examples from the Core-Excitation Spectra of CO<sub>2</sub> and N<sub>2</sub>O**, *Chem. Phys.* **13**, 153-160 (1976).

- 67 P.J. Bruna, S.D. Peyerimhoff and R.J. Buenker, **Calculation of the Vertical Electron Attachment Energy of Carbon Dioxide: Continuum States for Negative Ions**, *Chem. Phys. Letters* **39**, 211-216 (1976).
- 68 S.D. Peyerimhoff and R.J. Buenker, **Calculation of Potential Surfaces for Ground and Excited States**, in: *The New World of Quantum Chemistry*, edited by B. Pullman and R. Parr (Reidel, Dordrecht, 1976), pp. 213-240.
- 69 S.K. Shih, S.D. Peyerimhoff and R.J. Buenker, **Ab Initio Configuration Interaction Calculations for the Electronic Spectrum of Hydrogen Sulfide**, *Chem. Phys.* **17**, 391-402 (1976).
- 70 R.J. Buenker, S.D. Peyerimhoff and M. Perić, **Ab Initio Vibrational Analysis of the Schumann-Runge Bands and the Neighboring Absorption Region of Molecular Oxygen**, *Chem. Phys. Letters* **42**, 383-389 (1976).
- 71 J.G. Maas, N.P.F.B. van Asselt, P.J.C.M. Nowak, J. Los, S.D. Peyerimhoff and R.J. Buenker, **Ab Initio Calculations of the  $X^2\Sigma_u^+$  State of  $\text{He}_2^+$  and Adjustment Governed by Translational Spectroscopic Measurements**, *Chem. Phys.* **17**, 217-225 (1976).
- 72 B. Heß, P.J. Bruna, R.J. Buenker and S.D. Peyerimhoff, **Ab Initio CI Study of the Electronic Spectrum of Acetone**, *Chem. Phys.* **18**, 267-280 (1976).
- 73 S.K. Shih, S.D. Peyerimhoff and R.J. Buenker, **Theoretical Prediction of the Vertical Electronic Spectrum of the  $\text{C}_2\text{H}$  Radical**, *J. Mol. Spectrosc.* **64**, 167-179 (1977).
- 74 R.J. Buenker, S.K. Shih and S.D. Peyerimhoff, **All-Valence-Electron CI Treatment of the Electronic Spectrum of Trans-Butadiene**, *Chem. Phys. Letters* **44**, 385-393 (1976).
- 75 K.H. Thunemann, J. Römel, S.D. Peyerimhoff and R.J. Buenker, **A Study of the Convergence in Iterative Natural Orbital Procedures**, *Int. J. Quantum Chem.* **XI**, 743-752 (1977).
- 76 C. Marian, P.J. Bruna, R.J. Buenker and S.D. Peyerimhoff, **Comparison of the Structure and Spectra of the  $\text{HNO}^+$  and  $\text{NOH}^+$  Ions Using Ab Initio SCF and CI Methods**, *Mol. Phys.* **33**, 63-74 (1977).
- 77 A.B. Sannigrahi, K.H. Thunemann, S.D. Peyerimhoff and R.J. Buenker, **Ab Initio SCF and CI Study of the Ground and First Excited State of the HSO Radical**, *Chem. Phys.* **20**, 25-33 (1977).
- 78 S.K. Shih, S.D. Peyerimhoff and R.J. Buenker, **Theoretical Study of the Vertical Electronic Spectrum of  $\text{NO}_2$** , *Chem. Phys. Letters* **46**, 201-207 (1977).
- 79 A.B. Sannigrahi, S.D. Peyerimhoff and R.J. Buenker, **Non-empirical SCF and CI Study of the SOH Radical**, *Chem. Phys.* **20**, 381-389 (1977).

- 80 A. Richartz, R.J. Buenker, P.J. Bruna and S.D. Peyerimhoff, **Stability and Structure of the C<sub>2</sub>H<sub>6</sub><sup>+</sup> Ion: Investigation of the Photoelectron Spectrum of Ethane Below 14 eV Using Ab Initio Methods**, *Mol. Phys.* **33**, 1345-1366 (1977).
- 81 A.B. Sannigrahi, S.D. Peyerimhoff and R.J. Buenker, **Theoretical Study of the Geometry and Spectrum of the HS<sub>2</sub> Radical**, *Chem. Phys. Letters* **46**, 415-421 (1977).
- 82 M. Perić, R.J. Buenker and S.D. Peyerimhoff, **Theoretical Study of the Vibrational Structure of the <sup>1</sup>(n,π\*) Transition in Diimide: Potential Curves and Franck-Condon Analysis**, *Can. J. Chem.* **55**, 1533-1545 (1977).
- 83 R. Preuß, S.D. Peyerimhoff and R.J. Buenker, **Structure and Stability of the HFF and FHF Radicals**, *J. Mol. Struct.* **40**, 117-126 (1977).
- 84 P.J. Bruna, R.J. Buenker and S.D. Peyerimhoff, **Theoretical Prediction of the Electronic Spectrum of Thioacetone and Comparison with Related Systems**, *Chem. Phys.* **22**, 375-381 (1977).
- 85 R. Runau, S.D. Peyerimhoff and R.J. Buenker, **Ab Initio Study of the Photodissociation of Ammonia**, *J. Mol. Spectrosc.* **68**, 253-268 (1977).
- 86 M. Perić, S.D. Peyerimhoff and R.J. Buenker, **Ab Initio Calculation of the Vibrational Structure in the Electronic Spectra of HCN and DCN between 1700 and 2000 Å**, *Can. J. Chem.* **55**, 3664-3675 (1977).
- 87 J. Perić-Radić, J. Römel, S.D. Peyerimhoff and R.J. Buenker, **Configuration Interaction Calculation of the Potential Curves for the C<sub>3</sub> Molecule in its Ground and Lowest-lying Π<sub>u</sub> States**, *Chem. Phys. Letters* **50**, 344-350 (1977).
- 88 P.J. Bruna, S.D. Peyerimhoff and R.J. Buenker, **Ab Initio SCF and CI Study of the HCS<sup>+</sup>-CSH<sup>+</sup> System: Potential Surfaces for Hydrogen Abstraction and Internuclear Bending for Ground and Excited States and Vertical Spectrum for HCS<sup>+</sup>**, *Chem. Phys.* **27**, 33-43 (1978).
- 89 G. Hirsch, P.J. Bruna, S.D. Peyerimhoff and R.J. Buenker, **Ab Initio CI Study of the Stability and Electronic Spectrum of the HOCl Molecule**, *Chem. Phys. Letters* **52**, 442-448 (1977).
- 90 W. Butscher, R.J. Buenker and S.D. Peyerimhoff, **All-Electron CI Calculations for Core-Ionized, Core-valence Excited and Shake-up States of N<sub>2</sub>**, *Chem. Phys. Letters* **52**, 449-456 (1977).
- 91 W. Butscher, S.K. Shih, R.J. Buenker and S.D. Peyerimhoff, **Configuration Interaction Calculations for the N<sub>2</sub> Molecule and its Three Lowest Dissociation Limits**, *Chem. Phys. Letters* **52**, 457-462 (1977).

- 92 S.K. Shih, S.D. Peyerimhoff and R.J. Buenker, **MRD-CI Calculations for the Vertical Electronic Spectrum of the Hydroperoxyl Radical**, *Chem. Phys.* **28**, 299-304 (1978).
- 93 A. Richartz, R.J. Buenker and S.D. Peyerimhoff, **Ab Initio MRD-CI Study of Ethane: The 14-25 eV PES Region and Rydberg States of Positive Ions**, *Chem. Phys.* **28**, 305-312 (1978).
- 94 S.K. Shih, W. Butscher, R.J. Buenker and S.D. Peyerimhoff, **Calculation of the Vertical Electronic Spectrum of the Nitrogen Molecule Using the MRD-CI Method**, *Chem. Phys.* **29**, 241-252 (1978).
- 95 S.K. Shih, S.D. Peyerimhoff, R.J. Buenker and M. Perić, **Calculation of the Electron Affinity and  $^1\text{A}_1$ - $^3\text{B}_1$   $T_0$  Value of Methylene Using the Ab Initio MRDCI Method for a Large AO Basis**, *Chem. Phys. Letters* **55**, 206-212 (1978).
- 96 R.J. Buenker, S.D. Peyerimhoff and W. Butscher, **Applicability of the Multi-Reference Double-Excitation CI (MRD-CI) Method to the Calculation of Electronic Wavefunctions and Comparison with Related Techniques**, *Mol. Phys.* **35**, 771-791 (1978).
- 97 K.H. Thunemann, S.D. Peyerimhoff and R.J. Buenker, **Configuration Interaction Calculations for the Ground and Excited States of Ozone and Its Positive Ion: Energy Locations and Transition Probabilities**, *J. Mol. Spectrosc.* **70**, 432-448 (1978).
- 98 M. Perić, R.J. Buenker and S.D. Peyerimhoff, **Ab Initio CI Study of the Coupling of Small Vibrations in the Ground and  $^1\text{B}_{\text{g}}$  ( $n, \pi^*$ ) Excited States of  $\text{N}_2\text{H}_2$** , *Mol. Phys.* **35**, 1495-1498 (1978).
- 99 R. Preuß, R.J. Buenker and S.D. Peyerimhoff, **MRD-CI Calculations for the Structure and Stability of the HSiN-HNSi Isomers**, *J. Mol. Struct.* **49**, 171-179 (1978).
- 100 A. Richartz, R.J. Buenker and S.D. Peyerimhoff, **Calculation of the Vertical Electronic Spectrum of Propane**, *Chem. Phys.* **31**, 187-196 (1978).
- 101 J. Römelt, S.D. Peyerimhoff and R.J. Buenker, **Ab Initio MRDCI Calculations for the Electron Spectrum of the  $\text{C}_3$  Radical**, *Chem. Phys. Letters* **58**, 1-7 (1978).
- 102 M. Zeitz, S.D. Peyerimhoff and R.J. Buenker, **Theoretical Study of the Electronic Transition Moment for the  $d^3\Pi_{\text{g}}$ - $a^3\Pi_{\text{u}}$  Band System of the  $\text{C}_2$  Molecule**, *Chem. Phys. Letters* **58**, 487-491 (1978).
- 103 S.K. Shih, S.D. Peyerimhoff and R.J. Buenker, **Calculated Potential Surfaces for the Description of the Emission Spectrum of the  $\text{C}_2\text{H}$  Radical**, *J. Mol. Spectrosc.* **74**, 124-135 (1979).

- 104 R.J. Buenker and S.D. Peyerimhoff, **Accuracy, Timing and General Applicability of the MRD-CI Method**, in: *Excited States in Quantum Chemistry* (NATO ASI Series C46), edited by C.A. Nicolaides and D.R. Beck (Reidel, Dordrecht, 1979), pp.45-61.
- 105 R.J. Buenker, S.D. Peyerimhoff and M. Perić, **Calculation of Vibrational Wavefunctions and Energies Using MRD-CI Techniques**, in: *Excited States in Quantum Chemistry* (NATO ASI Series C46), edited by C.A. Nicolaides and D.R. Beck (Reidel, Dordrecht, 1979), pp. 63-77.
- 106 S.D. Peyerimhoff and R.J. Buenker, **CI Calculations of Vertical Excitation Energies and Oscillator Strengths for Rydberg and Valence States of Molecules**, in: *Excited States in Quantum Chemistry* (NATO ASI Series C46), edited by C.A. Nicolaides and D.R. Beck (Reidel, Dordrecht, 1979), pp. 79-103.
- 107 S.D. Peyerimhoff and R.J. Buenker, **Use of CI Methods for the Study of Molecular Dissociation Processes in Various Electronic States**, in: *Excited States in Quantum Chemistry* (NATO ASI Series C46), edited by C.A. Nicolaides and D.R. Beck (Reidel, Dordrecht, 1979), pp. 403-416.
- 108 R.J. Buenker, **Use of CI Methods for Approximate Solutions of the Global Schrödinger Equation**, *Gazz. Chim. Ital.* **108**, 245-252 (1978).
- 109 J. Römelt, S.D. Peyerimhoff and R.J. Buenker, **An SCF and MRD-CI Study of the Ground and Excited States of the He + H<sub>2</sub> System. I. Calculated Potential Surfaces**, *Chem. Phys.* **34**, 403-422 (1978).
- 110 R.J. Buenker, S.D. Peyerimhoff and S.K. Shih, **Comment on the Role of Configuration Selection Methods in Describing the V State of Ethylene**, *J. Chem. Phys.* **69**, 3882-3883 (1978).
- 111 K.H. Thunemann, R.J. Buenker, S.D. Peyerimhoff and S.K. Shih, **A Comparison of the Ethylene Ionization Potentials Obtained by the Green's Function Method and from CI Calculations**, *Chem. Phys.* **35**, 35-40 (1978).
- 112 R.J. Buenker, S.K. Shih and S.D. Peyerimhoff, **An MRD-CI Study of the Vertical 1(π,π\*) V-N Transition of Ethylene Using an AO Basis with Optimized Rydberg ndπ Species and Two Separate Carbon d Polarization Functions**, *Chem. Phys.* **36**, 97-111 (1979).
- 113 S.K. Shih, S.D. Peyerimhoff and R.J. Buenker, **Large Atomic Orbital Basis SCF and MRD-CI Calculations for Rearrangements of the PH<sub>5</sub> Molecule**, *J. Chem. Soc. Faraday Trans. II* **75**, 379-389 (1979).
- 114 R. Preuß, R.J. Buenker and S.D. Peyerimhoff, **Theoretical Study of the Electronically Excited States of the HNSi Molecule**, *Chem. Phys. Letters* **62**, 21-25 (1979).

- 115 P.J. Bruna, G. Hirsch, S.D. Peyerimhoff and R.J. Buenker, ***Ab Initio* SCF and CI Calculations for Ground and Low-lying Valence and Rydberg Excited States of HOCl and HClO in Linear and Bent Nuclear Conformations**, *Can. J. Chem.* **57**, 1839-1851 (1979).
- 116 M. Perić, R. Runau, J. Römelt, S.D. Peyerimhoff and R.J. Buenker, **Calculation of Wavefunctions and Frequencies for Non-infinitesimal Vibrations: Comparison of Various Methods Using *Ab Initio* CI Potential Curves**, *J. Mol. Spectrosc.* **78**, 309-332 (1979).
- 117 J. Römelt, S.D. Peyerimhoff and R.J. Buenker, **An SCF and MRD-CI Study of the Ground and Excited States of the He + H<sub>2</sub> System. II. Quenching of HD (1Σ<sub>u</sub><sup>+</sup>) Fluorescence and Other Energy Transfer Processes**, *Chem. Phys.* **41**, 133-141 (1979).
- 118 S.D. Peyerimhoff and R.J. Buenker, ***Ab Initio* MRD-CI Potential Surfaces for the Low-lying States of the NH<sub>2</sub><sup>+</sup> Molecular Ion**, *Chem. Phys.* **42**, 167-176 (1979).
- 119 M. Zeitz, S.D. Peyerimhoff and R.J. Buenker, **A Theoretical Study of the Bound Electronic States of the C<sub>2</sub><sup>-</sup> Negative Ion**, *Chem. Phys. Letters* **64**, 243-249 (1979).
- 120 M. Perić, R.J. Buenker and S.D. Peyerimhoff, ***Ab Initio* Configuration Interaction Study of the A<sup>2</sup>A<sub>1</sub>-X<sup>2</sup>B<sub>1</sub> Transition of PH<sub>2</sub> and PD<sub>2</sub>**, *Can. J. Chem.* **57**, 2491-2497 (1979).
- 121 S.D. Peyerimhoff and R.J. Buenker, **Potential Curves for Dissociative Electron Attachment of CFCl<sub>3</sub>**, *Chem. Phys. Letters* **65**, 434-439 (1979).
- 122 R.J. Buenker, P.J. Bruna and S.D. Peyerimhoff, ***Ab Initio* MRD-CI Calculations for HAB Molecules. I. Isomerization Energies for HOS, HNP and HCSi and their Positive Ions**, *Israel J. Chem.* **19**, 309-316 (1980).
- 123 V. Bonačić-Koutecký, R.J. Buenker and S.D. Peyerimhoff, **Use of Configuration Selection Methods to Study the Sudden Polarization Effect**, *J. Am. Chem. Soc.* **101**, 5917-5922 (1979).
- 124 S.D. Peyerimhoff and R.J. Buenker, **Theoretical Study of the X<sup>2</sup>B<sub>1</sub>, A<sup>2</sup>A<sub>1</sub>, <sup>2</sup>B<sub>2</sub> Valence-shell and the First π<sub>u</sub><sup>2</sup>3s-type Doublet and Quartet Rydberg States of NH<sub>2</sub>**, *Can. J. Chem.* **57**, 3182-3189 (1979).
- 125 S.D. Peyerimhoff and R.J. Buenker, **Calculation of Electronically Excited States in Molecules: Intensity and Vibrational Structure of Spectra, Photochemical Implications**, in: *Computational Methods in Chemistry*, edited by J. Bargon (Plenum, New York, 1980), pp. 175-202.
- 126 G. Hirsch, P.J. Bruna, R.J. Buenker and S.D. Peyerimhoff, **Non-adiabatic Coupling Matrix elements ⟨Ψ<sup>α</sup> | ∂/∂Q | Ψ<sup>β</sup>⟩ for Large CI Wavefunctions**, *Chem. Phys.* **45**, 335-347 (1980).

- 127 A. Barth, R.J. Buenker, S.D. Peyerimhoff and W. Butscher, **Theoretical Study of the Core-ionized and Various Core-excited and Shake-up States of Acetylene and Ethylene by *Ab Initio* MRD-CI Methods**, *Chem. Phys.* **46**, 149-164 (1980).
- 128 R.J. Buenker, S.D. Peyerimhoff and S.K. Shih, ***Ab Initio* Study of the Spatial Extension of the Ethylene V State**, *Chem. Phys. Letters* **69**, 7-13 (1980).
- 129 P.J. Bruna, S.D. Peyerimhoff and R.J. Buenker, **Theoretical Prediction of the Potential Curves for the Lowest-lying States of the Isovalent Diatomics  $\text{CN}^+$ ,  $\text{Si}_2$ ,  $\text{SiC}$ ,  $\text{CP}^+$  and  $\text{SiN}^+$ , Using the *Ab Initio* MRD-CI Method**, *J. Chem. Phys.* **72**, 5437-5445 (1980).
- 130 P.J. Bruna, G. Hirsch, M. Perić, S.D. Peyerimhoff and R.J. Buenker, **A Theoretical Study of the Lowest  ${}^2\text{B}_1$ ,  ${}^2\text{A}_1$  and  ${}^2\text{B}_2$  Electronic States in  $\text{H}_2\text{S}^+$  and a Comparison with Corresponding States in Related Systems**, *Mol. Phys.* **40**, 521-537 (1980).
- 131 K.H. Thunemann, R.J. Buenker and W. Butscher, **Configuration Interaction Study of the Electronic Spectrum of Furan**, *Chem. Phys.* **47**, 313-320 (1980).
- 132 S.D. Peyerimhoff and R.J. Buenker, **Application of the MRD-CI Method for the Prediction of Molecular Spectra and Properties**, in: Proceedings of the Workshop on *Quantum Chemistry and Molecular Physics*, edited by P.G. Burton (University of Wollongong Press, Wollongong/Australia, 1980).
- 133 R.J. Buenker, **The Configuration-Driven Table CI Method and Comparison with Integral-Driven CI Procedures**, in: Proceedings of the Workshop on *Quantum Chemistry and Molecular Physics*, edited by P.G. Burton (University of Wollongong Press, Wollongong/Australia, 1980).
- 134 P.J. Bruna, S.D. Peyerimhoff and R.J. Buenker, **The Ground State of the  $\text{CN}^+$  Ion: A Multi-reference CI Study**, *Chem. Phys. Letters* **72**, 278-284 (1980).
- 135 R.J. Buenker, V. Bonačić-Koutecký and L. Pogliani, **Potential Energy and Dipole Moment Surfaces for Simultaneous Torsion and Pyramidalization of Ethylene in its Lowest-lying Singlet Excited States: A CI Study of the Sudden Polarization Effect**, *J. Chem. Phys.* **73**, 1836-1849 (1980).
- 136 R.J. Buenker, S.D. Peyerimhoff and P.J. Bruna, **Development of a Computational Strategy in Electronic Structure Calculations: Error Analysis in CI Treatments**, in: *Computational Theoretical Organic Chemistry* (NATO ASI Series C67), edited by I.G. Csizmadia and R. Daudel (Reidel, Dordrecht, 1981), pp. 55-76.
- 137 J. Römel, S.D. Peyerimhoff and R.J. Buenker, ***Ab Initio* MRD-CI Study of the Rydberg States of Methylene**, *Chem. Phys.* **54**, 147-158 (1981).
- 138 P.J. Bruna, G. Hirsch, S.D. Peyerimhoff and R.J. Buenker, **Non-empirical CI Potential Curves for the Ground and Excited States of  $\text{PH}$  and its Positive Ion**, *Mol. Phys.* **42**, 875-898 (1981).

- 139 P.J. Bruna, G. Hirsch, R.J. Buenker and S.D. Peyerimhoff, **MRD-CI Method for the Study of Low-lying Electronic States. Application to Second-row Molecular Ions of Type  $AH_2^+$ ,  $AH^+$ ,  $AB^+$  and  $HAB^+$** , in: *Molecular Ions: Geometric and Electronic Structures* (NATO ASI Series B90), edited by J. Berkowitz and K.-O. Groeneveld (Plenum, New York, 1983), pp. 309-354.
- 140 J.S. Wright, S.K. Shih and R.J. Buenker, ***Ab Initio* Potential Surface for Ozone Decomposition**, *Chem. Phys. Letters* **75**, 513-518 (1980).
- 141 C. Petrongolo, P.J. Bruna, S.D. Peyerimhoff and R.J. Buenker, **Theoretical Prediction of the Potential Curves for the Lowest-lying States of the  $C_2^+$  Molecular Ion**, *J. Chem. Phys.* **74**, 4594-4602 (1981).
- 142 P.J. Bruna, C. Petrongolo, R.J. Buenker and S.D. Peyerimhoff, **Theoretical Prediction of the Potential Curves for the Lowest-lying States of the  $CSi^+$  and  $Si_2^+$  Molecular Ions**, *J. Chem. Phys.* **74**, 4611-4620 (1981).
- 143 M. Perić, S.D. Peyerimhoff and R.J. Buenker, ***Ab Initio* CI Calculation of the Band Structure in the  $A^2B_1$ - $X^2A_1$  Electronic Transition of  $BH_2$** , *Can. J. Chem.* **59**, 1318-1327 (1981).
- 144 R.J. Buenker, M. Perić, S.D. Peyerimhoff and R. Marian, ***Ab Initio* Treatment of the Renner-Teller Effect for the  $X^2B_1$  and  $A^2A_1$  Electronic States of  $NH_2$** , *Mol. Phys.* **43**, 987-1014 (1981).
- 145 S.D. Peyerimhoff and R.J. Buenker, **Electronically Excited and Ionized States of the Chlorine Molecule**, *Chem. Phys.* **57**, 279-296 (1981).
- 146 R.J. Buenker and V. Bonačić-Koutecký, **Determination of Properties of Close-lying Excited States of Olefins**, in: *Energy Storage and Redistribution in Molecules*, edited by J. Hinze (Plenum, New York, 1983), pp. 241-260.
- 147 G. Theodorakopoulos, S.D. Peyerimhoff and R.J. Buenker, ***Ab Initio* Configuration Interaction Study of the  $X^3\Sigma^-$ ,  $a^1\Delta$  and  $b^1\Sigma^+$  States of  $SO$  and  $S_2$** , *Chem. Phys. Letters* **81**, 413-420 (1981).
- 148 G.C. Lie, S.D. Peyerimhoff and R.J. Buenker, **Theoretical Dipole Derivatives for  $HCN$  and  $DCN$** , *J. Chem. Phys.* **75**, 2892-2898 (1981).
- 149 C.F. Chabalowski, R.J. Buenker and S.D. Peyerimhoff, **Theoretical Study of the Electronic Transition Moments for the  $d^3\Pi_g$  -  $a^3\Pi_u$  (Swan) and  $e^3\Pi_g$  -  $a^3\Pi_u$  (Fox-Herzberg) Bands in  $C_2$** , *Chem. Phys. Letters* **83**, 441-448 (1981).
- 150 M. Bettendorff, R.J. Buenker, S.D. Peyerimhoff and J. Römel, ***Ab Initio* CI Calculation of the Effects of Rydberg-Valence Mixing in the Electronic Spectrum of the HF Molecule**, *Z. Phys. A* **304**, 125-135 (1982).

- 151 M. Bettendorff, S.D. Peyerimhoff and R.J. Buenker, **Clarification of the Assignment of the Electronic Spectrum of Hydrogen Chloride Based on *Ab Initio* CI Calculations**, *Chem. Phys.* **66**, 261-279 (1982).
- 152 G.C. Lie, S.D. Peyerimhoff and R.J. Buenker, **Theoretical Integrated Intensities for the  $2\nu_2$  and  $2\nu_2 - \nu_2$  Bands of HCN and DCN**, *J. Mol. Spectrosc.* **93**, 74-82 (1982).
- 153 C. Petrongolo, R.J. Buenker and S.D. Peyerimhoff, **Nonadiabatic Treatment of the Intensity Distribution in the V-N Bands of Ethylene**, *J. Chem. Phys.* **76**, 3655-3667 (1982).
- 154 R.J. Buenker, **Implementation of the Table CI Method: Configurations Differing by Two in the Number of Open Shells**, in: *Current Aspects of Quantum Chemistry 1981* (Studies in Physical and Theoretical Chemistry, Vol. 21), edited by R. Carbó (Elsevier, Amsterdam, 1982), pp. 17-34.
- 155 R.J. Buenker, G. Hirsch, S.D. Peyerimhoff, P.J. Bruna, J. Römel, M. Bettendorff and C. Petrongolo, **Calculation of First- and Second-Derivative Non-adiabatic Matrix Elements with Large-scale CI Wavefunctions**, in: *Current Aspects of Quantum Chemistry 1981* (Studies in Physical and Theoretical Chemistry, Vol. 21), edited by R. Carbó (Elsevier, Amsterdam, 1982), pp. 81-97.
- 156 S.D. Peyerimhoff, P.S. Skell, D.D. May and R.J. Buenker, **Configuration Interaction Study of the Three Lowest Electronic States in the  $\text{HCO}_2$  and  $\text{CH}_3\text{CO}_2$  Radicals**, *J. Am. Chem. Soc.* **104**, 4515-4520 (1982).
- 157 C.M. Marian, R. Marian, S.D. Peyerimhoff, B.A. Heß, R.J. Buenker and G. Seger, ***Ab Initio* CI Calculation of  $\text{O}_2^+$  Predissociation Phenomena Induced by a Spin-orbit Coupling Mechanism**, *Mol. Phys.* **46**, 779-810 (1982).
- 158 G. Theodorakopoulos, C.A. Nicolaides, R.J. Buenker and S.D. Peyerimhoff, **Potential Energy Surfaces for the Photodissociation  $\text{H}_2\text{O} \rightarrow \text{O}(^1\text{D}_g) + \text{H}_2 (^1\Sigma_g^+)$** , *Chem. Phys. Letters* **89**, 164-170 (1982).
- 159 B.A. Heß, R.J. Buenker, C.M. Marian and S.D. Peyerimhoff, **Investigation of Electron Correlation on the Theoretical Prediction of Zero-field Splittings of  ${}^2\Pi$  Molecular States**, *Chem. Phys. Letters* **89**, 459-462 (1982).
- 160 B.A. Heß, R.J. Buenker, C.M. Marian and S.D. Peyerimhoff, ***Ab Initio* Calculation of the Zero-field Splittings of the  $\text{X}^3\Sigma_g^+$  and  $\text{B}^3\Pi_{g,i}$  States of the  $\text{S}_2$  Molecule**, *Chem. Phys.* **71**, 79-85 (1982).
- 161 S.D. Peyerimhoff and R.J. Buenker, **Potential Energy Curves and Transition Moments for the Low-lying Electronic States of the  $\text{Si}_2$  Molecule**, *Chem. Phys.* **72**, 111-118 (1982).

- 162 R.J. Buenker and S.D. Peyerimhoff, ***Ab Initio Calculations Close to the Full CI Level of Accuracy and their Use for the Interpretation of Molecular Spectra***, in: *New Horizons of Quantum Chemistry*, edited by P.-O. Löwdin and B. Pullman (Reidel, New York, 1983), pp. 183-219.
- 163 P.G. Burton, S.D. Peyerimhoff and R.J. Buenker, **Theoretical Studies of the Electronic Spectrum of Thioformaldehyde**, *Chem. Phys.* **73**, 83-98 (1982).
- 164 J. Anglada, P.J. Bruna, S.D. Peyerimhoff and R.J. Buenker, **MRD-CI Calculations for the Low-lying Electronic States of Scandium Hydride and Titanium Hydride**, *J. Mol. Struct. THEOCHEM* **93**, 299-308 (1983).
- 165 P.J. Bruna, H. Dohmann, J. Anglada, V. Krumbach, S.D. Peyerimhoff and R.J. Buenker, **The Relative Stability of  $^2\Sigma^+$  and  $^2\Pi$  States in the Systems  $\text{CSi}^-$ ,  $\text{Si}_2^-$ ,  $\text{SiP}$  and  $\text{P}_2^+$  as Predicted in MRD-CI Calculations**, *J. Mol. Struct. THEOCHEM* **93**, 309-318 (1983).
- 166 M. Lewerenz, P.J. Bruna, S.D. Peyerimhoff and R.J. Buenker, ***Ab Initio* MRD-CI Study of the Electronic Spectrum of  $\text{SiH}$** , *Mol. Phys.* **49**, 1-24 (1983).
- 167 M. Perić, S.D. Peyerimhoff and R.J. Buenker, **Use of the Vibronic CI Method in Accurate Calculations of the Renner-Teller Effect**, *Mol. Phys.* **49**, 379-400 (1983).
- 168 R. Klotz, C.M. Marian, S.D. Peyerimhoff, B.A. Heß and R.J. Buenker, **Study of the Dependence of Spin-orbit Matrix Elements on AO Basis Set Composition for Inner and Valence Shells: Results for the Multiplet Splitting of  $\text{X}^3\Sigma^-$  and  $\text{C}^3\Pi$  of SO and  $\text{X}^2\Pi$  in  $\text{SO}^+$** , *Chem. Phys.* **76**, 367-383 (1983).
- 169 C. Petrongolo, R.J. Buenker and S.D. Peyerimhoff, **Nonadiabatic Investigation of the V-N Spectrum of Ethylene in a New Diabatic Representation**, *J. Chem. Phys.* **78**, 7284-7289 (1983).
- 170 P. Chandra and R.J. Buenker, **Relativistic Integrals over Breit-Pauli Operators Using General Cartesian Gaussian Functions. I. One-electron Interactions**, *J. Chem. Phys.* **79**, 358-365 (1983).
- 171 P. Chandra and R.J. Buenker, **Relativistic Integrals over Breit-Pauli Operators Using General Cartesian Gaussian Functions. II. Two-Electron Interactions**, *J. Chem. Phys.* **79**, 366-372 (1983).
- 172 P.G. Burton, R.J. Buenker, P.J. Bruna and S.D. Peyerimhoff, **Comparison of Perturbatively Corrected MRD-CI Results with a Full CI Treatment of the BH Ground State**, *Chem. Phys. Letters* **95**, 379-385 (1983).
- 173 J. Anglada, P.J. Bruna, S.D. Peyerimhoff and R.J. Buenker, **Low-lying Electronic States of  $\text{CSi}^-$  and Electron Affinity of  $\text{CSi}$  According to *Ab Initio* MRD-CI Calculations**, *J. Phys. B: At. Mol. Phys.* **16**, 2469-2484 (1983).

- 174 M. Perić, S.D. Peyerimhoff and R.J. Buenker, **An *Ab Initio* Study of the A<sup>2</sup>A'-X<sup>2</sup>A'' Vibronic Transition in the Free Radical HNF**, *Can. J. Chem.* **61**, 2500-2505 (1983).
- 175 C.F. Chabalowski, S.D. Peyerimhoff and R.J. Buenker, **The Ballik-Ramsay, Mulliken, Deslandres-D'Azambuja and Phillips System in C<sub>2</sub>: A Theoretical Study of their Electronic Transition Moments**, *Chem. Phys.* **81**, 57-72 (1983).
- 176 J. Anglada, P.J. Bruna, S.D. Peyerimhoff and R.J. Buenker, **Comparison between Isoelectronic Transition Metal Hydrides. MRD-CI Results for ScH<sup>+</sup> and TiH<sup>+</sup>**, *J. Mol. Struct. THEOCHEM* **107**, 163-168 (1984).
- 177 M. Lewerenz, P.J. Bruna, S.D. Peyerimhoff and R.J. Buenker, **Ab Initio MRD-CI Calculation of the Electron Affinities of Si and SiH: Study of Three Stable States of the Respective Negative Ions**, *J. Phys. B: At. Mol. Phys.* **16**, 4511-4528 (1983).
- 178 M. Perić, M. Mladenović, S.D. Peyerimhoff and R.J. Buenker, **Ab Initio Study of the Isomerization HNC → HCN. I. Ab Initio Calculation of the HNC ↔ HCN Potential Surface and the Corresponding Energy Levels**, *Chem. Phys.* **82**, 317-336 (1983).
- 179 M. Bettendorff, R.J. Buenker and S.D. Peyerimhoff, **Investigation of Negative Ion States in HCl and HF by Configuration Interaction Methods**, *Mol. Phys.* **50**, 1363-1380 (1983).
- 180 H. Dohmann, P.J. Bruna, S.D. Peyerimhoff and R.J. Buenker, **Electronic Structure of the SiP<sup>+</sup> Radical on the Basis of Ab Initio MRD-CI Calculations**, *Mol. Phys.* **51**, 1109-1134 (1984).
- 181 G. Theodorakopoulos, S.C. Farantos, R.J. Buenker and S.D. Peyerimhoff, **MRD-CI Calculations on the Potential Energy Curves of the Ground and Excited Electronic States of the Noble-gas Hydrides, HeH, NeH and ArH**, *J. Phys. B: At. Mol. Phys.* **17**, 1453-1462 (1984).
- 182 R.J. Buenker, P. Chandra and B.A. Heß, **Matrix Representation of the Relativistic Kinetic Energy Operator: Two-component Variational Procedure for the Treatment of Many-electron Atoms and Molecules**, *Chem. Phys.* **84**, 1-9 (1984).
- 183 R.A. Phillips, R.J. Buenker, P.J. Bruna and S.D. Peyerimhoff, **Approaching the Full CI Limit with MRD-CI Calculations: The X<sup>1</sup>A<sub>1</sub> State of Water with a Double-zeta Basis**, *Chem. Phys.* **84**, 11-19 (1984).
- 184 M. Perić, S.D. Peyerimhoff and R.J. Buenker, **Ab Initio Study of the Renner-Teller Effect in the <sup>1</sup>Δ<sub>g</sub> State of CH<sub>2</sub>**, *Chem. Phys. Letters* **105**, 44-48 (1984).
- 185 M. Perić, R.J. Buenker and S.D. Peyerimhoff, **Ab Initio Study of the Vibronic Structure in the <sup>1</sup>Δ<sub>g</sub> State of NH<sub>2</sub><sup>+</sup>**, *Astrophys. Letters* **24**, 69-73 (1984).

- 186 R.J. Buenker, G. Olbrich, H.-P. Schuchmann, B.L. Schürmann and C. von Sonntag, **Photolysis of Methanol at 185 nm. Quantum Mechanical Calculations and Product Study**, *J. Am. Chem. Soc.* **106**, 4362-4368 (1984).
- 187 G. Theodorakopoulos, I.D. Petsalakis, R.J. Buenker and S.D. Peyerimhoff, **Bending Potentials for H<sub>2</sub>O in the Ground and the First Six Singlet Excited States**, *Chem. Phys. Letters* **105**, 253-257 (1984).
- 188 M. Perić, M. Mladenović, S.D. Peyerimhoff and R.J. Buenker, **Ab Initio Study of the HNC → HCN Isomerization. II. Calculation of the Isomerization Rate Constant**, *Chem. Phys.* **86**, 85-103 (1984).
- 189 J.S. Wright and R.J. Buenker, **The Effect of Bond Functions on Molecular Dissociation Energies**, *Chem. Phys. Letters* **106**, 570-574 (1984).
- 190 B.A. Heß, P. Chandra and R.J. Buenker, **Ab Initio Calculation of the Ground State and the First Excited State System of Br Including Spin-orbit Coupling and Relativistic Correction to the Kinetic Energy Operator**, *Mol. Phys.* **52**, 1177-1190 (1984).
- 191 R.J. Buenker, B.A. Heß and P. Chandra, **Reply to the Comments of Jan Almlöf, Knut Faegri, and Hans H. Grelland and Alfredo Simas and Vedene H. Smith, Jr.**, *J. Chem. Phys.* **80**, 6330-6331 (1984).
- 192 I.D. Petsalakis, G. Theodorakopoulos, C.A. Nicolaides, R.J. Buenker and S.D. Peyerimhoff, **Nonorthonormal CI for Molecular Excited States. I. The Sudden Polarization Effect in 90° Twisted Ethylene**, *J. Chem. Phys.* **81**, 3161-3167 (1984).
- 193 R. Klotz, C.M. Marian, S.D. Peyerimhoff, B.A. Heß and R.J. Buenker, **Calculation of Spin-forbidden Radiative Transitions Using Correlated Wavefunctions: Lifetime of b<sup>1</sup>Σ<sup>+</sup>, a<sup>1</sup>Δ States in O<sub>2</sub>, S<sub>2</sub> and SO**, *Chem. Phys.* **89**, 223-236 (1984).
- 194 M. Perić, R.J. Buenker and S.D. Peyerimhoff, **Theoretical Study of the U.V. Spectrum of Acetylene. I. Ab Initio Calculation of Singlet Electronic States of Acetylene by a Large-scale CI method**, *Mol. Phys.* **53**, 1177-1193 (1984).
- 195 F. Grein, S.D. Peyerimhoff and R.J. Buenker, **Ab Initio Studies on the Oscillator Strength of the 2<sup>3</sup>Π<sub>u</sub>-X<sup>1</sup>Σ<sub>g</sub><sup>+</sup> Spin-forbidden Transition in Cl<sub>2</sub>**, *Can. J. Phys.* **62**, 1928-1932 (1984).
- 196 I.D. Petsalakis, G. Theodorakopoulos, C.A. Nicolaides and R.J. Buenker, **Non-orthonormal CI for Molecular Excited States. II. The Zwitterionic States of Terminally Twisted Butadiene**, *J. Chem. Phys.* **81**, 5952-5956 (1984).
- 197 F. Grein, S.D. Peyerimhoff and R.J. Buenker, **Theoretical Studies on Excited States of Ne<sub>2</sub>. I. MRD-CI Potential Energy Curves**, *J. Chem. Phys.* **82**, 353-363 (1985).

- 198 G. Theodorakopoulos, I.D. Petsalakis, C.A. Nicolaides and R.J. Buenker, **The  $\tilde{X}^1A_1$ - $\tilde{A}^1B_1$  Transition Moment of  $H_2O$  Using State-specific Configuration-Interaction Wave Functions**, *J. Chem. Phys.* **82**, 912-916 (1985).
- 199 P.R. Bunker, R.A. Phillips and R.J. Buenker, **An *Ab Initio* Study of the Rotation-Vibration Energy Levels of  $GeH_2$  in the  $\tilde{X}^1A_1$  State**, *Chem. Phys. Letters* **110**, 351-355 (1984).
- 200 G. Hirsch and R.J. Buenker, ***Ab Initio* MRD-CI Study of  $NO_2$ . 1. Multi-dimensional Potential Surfaces for the Two Lowest  $^2A'$  States**, *Can. J. Chem.* **63**, 1542-1549 (1985).
- 201 R.J. Buenker and R.A. Phillips, **Implementation of the Table CI Method: Matrix Elements between Configurations with the Same Number of Open Shells**, *J. Mol. Struct. THEOCHEM* **123**, 291-300 (1985).
- 202 G.C. Lie, S.D. Peyerimhoff and R.J. Buenker, **Configuration Interaction Studies of Low-lying Valence and Rydberg States of NS**, *J. Chem. Phys.* **82**, 2672-2678 (1985).
- 203 G. Theodorakopoulos, I.D. Petsalakis and R.J. Buenker, **MRD-CI Calculations on the Asymmetric Stretch Potentials of  $H_2O$  in the Ground and the First Seven Singlet Excited States**, *Chem. Phys.* **96**, 217-225 (1985).
- 204 C. Petrongolo, R.J. Buenker and S.D. Peyerimhoff, **Potential Surfaces and Vibronic Coupling for the Conical Intersection of the  $\tilde{A}^2A_1$  and  $\tilde{B}^2B_2$  States of  $NH_2$** , *Chem. Phys. Letters* **115**, 249-252 (1985).
- 205 M. Perić, S.D. Peyerimhoff and R.J. Buenker, ***Ab Initio* Treatment of the Renner-Teller Effect and Application to Various  $AH_2$  and HAB Molecules**, *Int. Rev. Phys. Chem.* **4**, 85-124 (1985).
- 206 G.J. Vazquez, S.D. Peyerimhoff and R.J. Buenker, **MRD-CI Study of the Photodissociation of  $HO_2$  into  $OH(X^2\Pi) + O(^3P, ^1D)$** , *Chem. Phys.* **99**, 239-257 (1985).
- 207 M. Perić, S.D. Peyerimhoff and R.J. Buenker, **Theoretical Study of the U.V. Spectrum of Acetylene. II. *Ab Initio* Treatment of the Renner-Teller Effect in  $^1\Pi_u$  and  $^1\Delta_g$  Electronic States**, *Mol. Phys.* **55**, 1129-1145 (1985).
- 208 B.L. Schürmann and R.J. Buenker, ***Ab Initio* SCF and MRD-CI Description of the  $A^2A'-X^2A''$  Transition of the as yet Unknown  $HNCl$  Molecule**, *Can. J. Chem.* **63**, 3264-3268 (1985).
- 209 R.A. Phillips, R.J. Buenker, R. Beardsworth, P.R. Bunker, P. Jensen and W.P. Kraemer, **An *Ab Initio* Study of the Rotation-Vibration Energy Levels of  $GeH_2$  in the  $\tilde{a}^3B_1$  State**, *Chem. Phys. Letters* **118**, 60-63 (1985).
- 210 R.J. Buenker, Book Review of **Physical Sciences Data 16, Gaussian Basis Sets for Molecular Calculations**, by S. Huzinaga et al., *Theor. Chim. Acta* **67**, 337 (1985).

- 211 B.A. Heß, P. Chandra and R.J. Buenker, ***Ab Initio* MRD-CI Calculation of the Zero-Field Splitting of the  $^2\Pi$  Ground State of the CBr Molecule**, *Chem. Phys. Letters* **119**, 403-406 (1985).
- 212 J.S. Wright and R.J. Buenker, **MRD-CI Potential Surfaces Using Balanced Basis Sets. III. HCl and N<sub>2</sub>**, *J. Chem. Phys.* **83**, 4059-4068 (1985).
- 213 C.F. Chabalowski, R.J. Buenker and S.D. Peyerimhoff, ***Ab Initio* Study of the Locations and Intensities of the Lowest-lying Electronic Transitions of the C<sub>3</sub> and C<sub>2</sub>O Molecules**, *J. Chem. Phys.* **84**, 268-274 (1986).
- 214 G. Theodorakopoulos, I.D. Petsalakis, C.A. Nicolaides and R.J. Buenker, **Configuration Interaction Study of the Oscillator Strengths for the  $\tilde{B}^1A_1$  -  $\tilde{X}^1A_1$  and  $\tilde{D}^1A_1$  -  $\tilde{X}^1A_1$  Transitions of the Water Molecule**, *Chem. Phys.* **100**, 331-337 (1985).
- 215 B.A. Heß and R.J. Buenker, ***Ab Initio* MRD-CI Potential Curves, Dipole Moments and Zero-field Splittings for the X $^2\Pi$  Ground States of the CF and CCl Molecules**, *Chem. Phys.* **101**, 211-218 (1986).
- 216 R.J. Buenker, **Combining Perturbation Theory Techniques with Variational CI Calculations to Study Molecular Excited States**, *Int. J. Quantum Chem.* **XXIX**, 435-460 (1986).
- 217 B.A. Heß, R.J. Buenker and P. Chandra, **Toward the Variational Treatment of Spin-orbit and Other Relativistic Effects for Heavy Atoms and Molecules**, *Int. J. Quantum Chem.* **XXIX**, 737-753 (1986).
- 218 R.J. Buenker, ***Ab Initio* MRD-CI Calculations for the Decay of Molecular Excited States Via Radiative and Dissociative Mechanisms**, *J. Mol. Struct. THEOCHEM* **149**, 1-21 (1987).
- 219 G.J. Vazquez, R.J. Buenker and S.D. Peyerimhoff, **The Electronic Structure of HO<sub>2</sub><sup>+</sup>: An MRD-CI Study**, *Mol. Phys.* **59**, 291-316 (1986).
- 220 M. Perić, B.A. Heß and R.J. Buenker, ***Ab Initio* Study of the Renner-Teller Effect and Spin-orbit Coupling in the X $^2\Pi$  Ground State of NCO**, *Mol. Phys.* **58**, 1001-1011 (1986).
- 221 M. Perić, R.J. Buenker and S.D. Peyerimhoff, **Use of Trigonometric Series for Solution of the Schrödinger Equation for Bending Vibrations in Triatomic Molecules**, *Mol. Phys.* **59**, 1283-1303 (1986).
- 222 C. Marian, B.A. Heß, S. Schöttke and R.J. Buenker, **Is There a Stable B $^2\Pi$  State for the CNO Molecule?** *J. Mol. Spectrosc.* **124**, 190-198 (1987).

- 223 M. Perić, H. Dohmann, S.D. Peyerimhoff and R.J. Buenker, **Potential Surfaces for Valence-Type Singlet Electronic States of the HCN Molecule**, *Z. Phys. D: Atoms, Molecules and Clusters* **5**, 65-75 (1987).
- 224 G. Theodorakopoulos, I.D. Petsalakis, C.A. Nicolaides and R.J. Buenker, **Theoretical Dipole Transition Moments for the Transitions to the Ground State  $X^2\Sigma^+$  from the  $A^2\Sigma^+$ ,  $B^2\Pi$ ,  $C^2\Sigma^+$ ,  $D^2\Sigma^+$  and  $E^2\Pi$  States and for the  $B^2\Pi \rightarrow A^2\Sigma^+$  System in HeH**, *J. Phys. B: At. Mol. Phys.* **20**, 2339-2345 (1987).
- 225 G. Theodorakopoulos, I.D. Petsalakis, C.A. Nicolaides and R.J. Buenker, **Non-orthonormal Basis Calculations of the Dipole Transition Moment for the Phillips System ( $A^1\Pi_u \rightarrow X^1\Sigma_g^+$ ) in  $C_2$ . Theoretical Lifetime of the  $A^1\Pi_u$  State**, *Chem. Phys.* **112**, 319-324 (1987).
- 226 R.A. Phillips and R.J. Buenker, **Factors Involved in the Accurate Calculation of Oscillator Strengths: The  $A^1B_1$ - $X^1A_1$  Transition of  $H_2O$** , *Chem. Phys. Letters* **137**, 157-161 (1987).
- 227 A. Metropoulos, C.A. Nicolaides and R.J. Buenker, **Adiabatic Calculations of the  $^2\Sigma_g^+$  Excited States of  $He_2^+$** , *Chem. Phys.* **114**, 1-7 (1987).
- 228 J.S. Wright, V.J. Barclay and R.J. Buenker, **Bond Functions in Molecular Excited States: MRD-CI Calculations for the  $A^3\Sigma_u^+$ ,  $B^3\Pi_g$  and  $W^3\Delta_u$  States of  $N_2$** , *Chem. Phys.* **115**, 23-32 (1987).
- 229 G. Theodorakopoulos, I.D. Petsalakis and R.J. Buenker, **Theoretical Investigation of the Character of the Electronic States of  $H_2O$  along a Linear Dissociation Path Leading to OH+H**, *Chem. Phys. Letters* **138**, 71-75 (1987).
- 230 P.R. Bunker, D.B. Knowles, B.L. Schürmann and R.J. Buenker, **The *Ab Initio* Calculation of the Band Origin and Vibrational Frequencies of the  $\tilde{A}$  -  $\tilde{X}$  System of HNCl Using the Non-rigid Bender Hamiltonian**, *Chem. Phys. Letters* **139**, 159-164 (1987).
- 231 G. Theodorakopoulos, I.D. Petsalakis and R.J. Buenker, **Theoretical Investigation of the Excited States of NeH: Calculations of Dipole Transition Moments and Radial Coupling Matrix Elements**, *J. Phys. B: At. Mol. Phys.* **20**, 5335-5344 (1987).
- 232 I.D. Petsalakis, G. Theodorakopoulos, C.A. Nicolaides and R.J. Buenker, **Theoretical Dipole Transition Moments for Transitions between Bound Electronic States and Non-adiabatic Coupling Matrix Elements between  $^2\Sigma^+$  of HeH**, *J. Phys. B: At. Mol. Phys.* **20**, 5959-5965 (1987).
- 233 M. Perić, R.J. Buenker and S.D. Peyerimhoff, **Theoretical Study of the Vibronic Structure of the  $1^1\Pi \leftarrow X^1\Sigma^+$  Electronic Transition in HCN and DCN**, *Mol. Phys.* **62**, 1323-1338 (1987).

- 234 G. Hirsch and R.J. Buenker, **Theoretical Study of the Properties of BC and Its Positive Ion in Their Ground and Excited Electronic States**, *J. Chem. Phys.* **87**, 6004-6011 (1987).
- 235 M. Perić, S.D. Peyerimhoff and R.J. Buenker, **Theoretical Study of the U.V. Spectrum of Acetylene. III. Ab Initio Investigation of the Valence-Type Singlet Electronic States**, *Mol. Phys.* **62**, 1339-1356 (1987).
- 236 T. Fueno and R.J. Buenker, **Electronic Structures of the S<sub>2</sub>O and S<sub>3</sub> Isomers: An Ab Initio CI Study**, *Theor. Chim. Acta* **73**, 123-134 (1988).
- 237 R.J. Buenker and P. Chandra, **Application of Configuration Interaction for the Study of Relativistic Effects in Atoms and Molecules**, *Pure Appl. Chem.* **60**, 167-173 (1988).
- 238 J.R. Alvarez-Collado and R.J. Buenker, **Theoretical Study of the Transition Probabilities among the Three Lowest Electronic States of the SeS Molecule**, *Mol. Phys.* **64**, 725-738 (1988).
- 239 M. Perić, R.J. Buenker and S.D. Peyerimhoff, **Ab Initio CI Study of the Vibrational Structure of the 1<sup>1</sup>Σ-(1<sup>1</sup>A'') ← X and 1<sup>1</sup>Δ(2<sup>1</sup>A', 2<sup>1</sup>A'') ← X Electronic Transitions in HCN and DCN**, *Mol. Phys.* **64**, 843-864 (1988).
- 240 B.L. Schürmann, D.B. Knowles, G. Hirsch and R.J. Buenker, **An Ab Initio CI Study of the Lowest Electronic States of the HPF Molecule**, *Chem. Phys. Letters* **145**, 529-536 (1988).
- 241 M. Perić, Bhanuprakash K. and R.J. Buenker, **Ab Initio MRD-CI Study of the Renner-Teller Effect and Spin-orbit Coupling in the X<sup>2</sup>Π<sub>g</sub> Ground State of BO<sub>2</sub>**, *Mol. Phys.* **65**, 403-412 (1988).
- 242 G.J. Vazquez, R.J. Buenker and S.D. Peyerimhoff, **MRD-CI Study of the Electron Affinity of HO<sub>2</sub> and the Photodetachment Energy of HO<sub>2</sub><sup>-</sup>**, *Chem. Phys.* **129**, 405-415 (1989).
- 243 G. Theodorakopoulos, I.D. Petsalakis and R.J. Buenker, **Non-adiabatic Interactions between the C<sup>2</sup>Σ<sup>+</sup> and D<sup>2</sup>Σ<sup>+</sup> Electronic States of HeH**, *Chem. Phys. Letters* **148**, 285-288 (1988).
- 244 I.D. Petsalakis, G. Theodorakopoulos and R.J. Buenker, **Radiative Dissociation and Predissociation in HeH and NeH: A Theoretical Treatment using Square-Integrable Functions**, *Phys. Rev. A* **38**, 4004-4008 (1988).
- 245 K. Bhanuprakash and R.J. Buenker, **Ab Initio Calculations of the Electronic Transition Moments and Radiative Lifetimes in some BN Band Systems**, *Chem. Phys. Letters* **152**, 215-221 (1988).

- 246 R.J. Buenker, D.B. Knowles, S.N. Rai, G. Hirsch, Bhanuprakash K. and J.R. Alvarez-Collado, **Use of Perturbative Corrections in MRD-CI Treatments and Comparison with Full CI Benchmark Results**, in: *Quantum Chemistry - Basic Aspects, Actual Trends* (Studies in Physical and Theoretical Chemistry, Vol. 62), edited by R. Carbó (Elsevier, Amsterdam, 1989), pp. 181-198.
- 247 G.J. Vazquez, R.J. Buenker and S.D. Peyerimhoff, **Multireference Singles and Doubles Configuration Interaction Study of the Photoelectron Spectrum of HO<sub>2</sub><sup>-</sup>**, *J. Chem. Phys.* **90**, 7229-7238 (1989).
- 248 Bhanuprakash K., P. Chandra, G. Hirsch and R.J. Buenker, **Ab Initio Calculations for Dipole-Forbidden Transitions in NBr: Radiative Lifetimes of the b<sup>1</sup>Σ<sup>+</sup> and a<sup>1</sup>Δ States**, *Chem. Phys.* **133**, 345-354 (1989).
- 249 H. Thümmel, M. Perić, S.D. Peyerimhoff and R.J. Buenker, **Ab Initio Calculation of the Potential Surfaces for Low-lying Valence Electronic States of the C<sub>2</sub>H Radical**, *Z. Phys. D: Atoms, Molecules and Clusters* **13**, 307-316 (1989).
- 250 G. Theodorakopoulos, I.D. Petsalakis, R.J. Buenker and M. Honigmann, **MRD-CI Calculations on the Radiative Lifetime of the A<sup>2</sup>Δ State of CH**, *Chem. Phys.* **137**, 137-141 (1989).
- 251 Bhanuprakash K., P. Chandra, C. Chabalowski and R.J. Buenker, **Theoretical Study of the Generalized Oscillator Strength for the A<sup>1</sup>B<sub>1</sub>-X<sup>1</sup>A<sub>1</sub> Transition in the Water Molecule**, *Chem. Phys.* **138**, 215-221 (1989).
- 252 D.B. Knowles, J.R. Alvarez-Collado, G. Hirsch and R.J. Buenker, **Comparison of Perturbatively Corrected Energy Results from Multiple Reference Double-excitation Configuration-Interaction Method Calculations with Exact Full Configuration-Interaction Benchmark Values**, *J. Chem. Phys.* **92**, 585-596 (1990).
- 253 I.D. Petsalakis, G. Theodorakopoulos and R.J. Buenker, **Theoretical Treatment of Predissociation in the A<sup>2</sup>Σ<sup>+</sup>, B<sup>2</sup>Π, and C<sup>2</sup>Σ<sup>+</sup> States of HeH**, *J. Chem. Phys.* **92**, 4920-4923 (1990).
- 254 P. Jensen, R.J. Buenker, G. Hirsch and S.N. Rai, **An Ab Initio Calculation of the Rotational-Vibrational Energies in the Electronic Ground State of NH<sub>2</sub>**, *Mol. Phys.* **70**, 443-454 (1990).
- 255 C. Petrongolo, G. Hirsch and R.J. Buenker, **Diabatic Representation of the Ā<sup>2</sup>A<sub>1</sub>/Ā<sup>2</sup>B<sub>2</sub> Conical Intersection in NH<sub>2</sub>**, *Mol. Phys.* **70**, 825-834 (1990).
- 256 G. Hirsch, R.J. Buenker and C. Petrongolo, **Ab Initio Study of NO<sub>2</sub>. Part II. Non-adiabatic Coupling between the Two Lowest <sup>2</sup>A' States and the Construction of a Diabatic Representation**, *Mol. Phys.* **70**, 835-848 (1990).

- 257 S.N. Rai, R.J. Buenker and G. Hirsch, **An *Ab Initio* CI Study of the Geometry and Spectrum of the HSe<sub>2</sub> Radical**, *Chem. Phys. Letters* **170**, 39-43 (1990).
- 258 M. Perić, R.J. Buenker and S.D. Peyerimhoff, ***Ab Initio* Investigation of the Vibronic Structure of the C<sub>2</sub>H Spectrum. II. Calculation of Diabatic Potential Surfaces for the Three Lowest-lying Electronic States in C<sub>2</sub>H**, *Mol. Phys.* **71**, 673-691 (1990).
- 259 M. Perić, S.D. Peyerimhoff and R.J. Buenker, ***Ab Initio* Investigation of the Vibronic Structure of the C<sub>2</sub>H Spectrum. III. Calculation of Vibronic Energies and Transition Probabilities in the X<sup>2</sup>Σ<sup>+</sup>, A<sup>2</sup>Π System**, *Mol. Phys.* **71**, 693-719 (1990).
- 260 S.N. Rai and R.J. Buenker, **Theoretical Prediction of the Radiative Lifetimes of the Two Lowest Excited Electronic States of TeO**, *Chem. Phys.* **147**, 327-333 (1990).
- 261 G. Theodorakopoulos, I.D. Petsalakis and R.J. Buenker, **Theoretical Calculations of the Rydberg Spectra of ArH**, *Mol. Phys.* **71**, 1055-1062 (1990).
- 262 S. Roszak, R.J. Buenker, P.C. Hariharan and J.J. Kaufman, ***Ab Initio* MRD CI Ground and Excited State Potential Curves for Addition of O to H<sub>2</sub>C=CH<sub>2</sub> and Oxirane Formation and Decomposition**, *Chem. Phys.* **147**, 13-18 (1990).
- 263 Bhanuprakash K., G. Hirsch and R.J. Buenker, **Dipole-forbidden Transitions in Se<sub>2</sub>: *Ab Initio* Calculations of the Radiative Lifetimes of the a<sup>1</sup>Δ<sub>g</sub> and b<sup>1</sup>Σ<sub>g</sub><sup>+</sup> States**, *Mol. Phys.* **72**, 1185-1192 (1990).
- 264 L. Chantranupong, G. Hirsch, R.J. Buenker, M. Kimura and M.A. Dillon, **Theoretical Study of the Electronic Spectrum of Ammonia: Generalized Oscillator Strength Calculations for the A-X Transition**, *Chem. Phys.* **154**, 13-21 (1991).
- 265 G. Hirsch, R.J. Buenker and C. Petrongolo, ***Ab Initio* Study of NO<sub>2</sub>. Part III. Potential Energy Functions for the Two Lowest 2A' States in Both the Diabatic and Adiabatic Representations**, *Mol. Phys.* **73**, 1085-1099 (1991).
- 266 M. Perić, S.D. Peyerimhoff and R.J. Buenker, ***Ab Initio* Investigation of the Vibronic Structure in the C<sub>2</sub>H Spectrum: Calculation of Vibronic Energies and Wavefunctions for Various Isotopomers**, *J. Mol. Spectrosc.* **148**, 180-200 (1991).
- 267 D.A. Chapman, S. Roszak, P.B. Keegstra, P.C. Hariharan, J.J. Kaufman and R.J. Buenker, ***Ab Initio* MRD-CI Calculations for Breaking a Chemical Bond in a Molecule in a Crystal or Other Solid Environment. III. Me<sub>2</sub>N-NO<sub>2</sub> Decomposition of Dimethylnitramine in a Large Crystalline Environment**, *Int. J. Quantum Chem.* **XXXIX**, 541-560 (1991).
- 268 D.A. Chapman, J.J. Kaufman and R.J. Buenker, ***Ab Initio* MRD-CI Calculations on Cubane (Neutral, Carbocation, Carboanion) and ≡C-NO<sub>2</sub> Dissociation of Nitrocubanes Based on Localized Orbitals**, *Int. J. Quantum Chem.* **XL**, 389-403 (1991).

- 269 J.R. Alvarez-Collado and R.J. Buenker, **On the Numerical Solution of the Multidimensional Vibrational Time-Independent Schrödinger Equation**, *J. Comput. Chem.* **13**, 135-141 (1992).
- 270 I.D. Petsalakis, G. Theodorakopoulos, C.A. Nicolaides and R.J. Buenker, **Nearly Diabatic States by Maximization of the Non-orthonormal Overlap between Model-diabatic and MRD-CI Wavefunctions**, *Chem. Phys. Letters* **185**, 359-364 (1991).
- 271 M. Honigmann, R.J. Buenker, G. Hirsch and S. Schöttke, **Calculation of Predissociation Resonances for the  $A^2\Sigma^+$  HeH with the Complex Coordinate Method in a Diabatic Hamiltonian Representation**, *J. Phys. B: At. Mol. Opt. Phys.* **25**, 389-398 (1992).
- 272 R.J. Buenker, **Evidence from the Special Relativity and Blackbody Radiation Theories for the Existence of Photons Possessing Zero Kinetic Energy**, *Mol. Phys.* **76**, 277-291 (1992); see also <http://arxiv.org/physics/0501054>.
- 273 L. Chantranupong, Bhanuprakash K., M. Honigmann, G. Hirsch and R.J. Buenker, **A Configuration Interaction Study of the Oscillator Strengths for Various Low-lying Transitions of the CO Molecule**, *Chem. Phys.* **161**, 351-362 (1992).
- 274 G. Hirsch, R.J. Buenker and C. Petrongolo, **On the Nature of the Reaction Path from the  $2B_2$  Stationary Point to the  $\tilde{X} \ 2A_1$  Minimum on the Lowest  $2A'$  Potential Energy Surface of NO<sub>2</sub>**, *Mol. Phys.* **76**, 1261-1263 (1992).
- 275 S.N. Rai and R.J. Buenker, **A Theoretical Investigation of the Lowest  $B_u$  State of *trans*-Butadiene**, *Indian J. Chem.* **31A**, 215-218 (1992).
- 276 Y. Li, M. Honigmann, Bhanuprakash K., G. Hirsch, R.J. Buenker, M.A. Dillon and M. Kimura, **Coupled Diabatic Configuration Interaction Treatment of the O<sub>2</sub> B'-X Transition Including Computation of Predissociation Linewidths, Optical f Values, and Generalized Oscillator Strengths**, *J. Chem. Phys.* **96**, 8314-8323 (1992).
- 277 L. Chantranupong, G. Hirsch, Bhanuprakash K., R.J. Buenker, M. Kimura and M.A. Dillon, **Ab Initio CI Calculation of the Generalized Oscillator Strength for Four Transitions of the CO Molecule**, *Chem. Phys.* **164**, 183-190 (1992).
- 278 M. Perić, S.D. Peyerimhoff and R.J. Buenker, **Analysis and Predictions of the Vibronic Spectrum of the Ethynyl Radical C<sub>2</sub>H by Ab Initio Methods**, *Z. Phys. D - Atoms, Molecules and Clusters* **24**, 177-198 (1992).
- 279 R.J. Buenker, **Exponentially Damped Breit-Pauli Hamiltonian for the Description of Positronium Decay and Other High-energy Processes**, *Mol. Phys.* **77**, 1095-1122 (1992); see also <http://arxiv.org/physics/0504070>.
- 280 A. Metropoulos, Y. Li, G. Hirsch and R.J. Buenker, **Electric Dipole Transition Moments between the  $2\Sigma_u^+$  and  $2\Sigma_g^+$  States of the He<sub>2</sub><sup>+</sup> Ion**, *Chem. Phys. Letters* **198**, 266-272 (1992).

- 281 L. Chantranupong, G. Hirsch, R.J. Buenker and M.A. Dillon, **Configuration Interaction Calculations of the Vertical Electronic Spectrum of Silane**, *Chem. Phys.* **170**, 167-175 (1993).
- 282 L. Chantranupong, G. Hirsch, R.J. Buenker and M.A. Dillon, **Theoretical Configuration Interaction Study of the Vertical Electronic Spectrum of Ethane**, *J. Mol. Struct.* **297**, 373-381 (1993).
- 283 M. Honigmann, G. Hirsch and R.J. Buenker, **Theoretical Study of the Optical and Generalized Oscillator Strengths for Transitions between Low-lying Electronic States of the BF Molecule**, *Chem. Phys.* **172**, 59-71 (1993).
- 284 Y. Li, S. Carter, G. Hirsch and R.J. Buenker, **Theoretical Calculation of the Potential Surfaces and Vibrational Frequencies of the  $A^2\Sigma^+$  and  $X^2\Pi$  Electronic States of the NCO Radical**, *Mol. Phys.* **80**, 145-152 (1993).
- 285 A.B. Alekseyev, H.-P. Liebermann, I. Boustani, G. Hirsch and R.J. Buenker, **Theoretical Study of the Energies and Lifetimes of the Low-lying States of Bismuth Fluoride**, *Chem. Phys.* **173**, 333-344 (1993).
- 286 M. Kimura, A. Dalgarno, L. Chantranupong, Y. Li, G. Hirsch and R.J. Buenker, **Rate Coefficients for Charge Transfer of  $\text{He}^+$  with C**, *Astrophys. J.* **417**, 812-814 (1993).
- 287 I. Boustani, S.N. Rai, H.-P. Liebermann, A.B. Alekseyev, G. Hirsch and R.J. Buenker, **Relativistic Configuration Interaction Calculations of Potential Curves and Radiative Transition Probabilities for the Antimony Fluoride Molecule**, *Chem. Phys.* **177**, 45-52 (1993).
- 288 Y. Li, M. Honigmann, G. Hirsch and R.J. Buenker, **Theoretical Study of Line Broadening in the  $(3s\sigma)$   $^3\Pi_g$  Vibrational Levels of the  $\text{O}_2$  Molecule Employing a Diabatic CI Representation**, *Chem. Phys. Letters* **212**, 185-192 (1993).
- 289 H.-P. Liebermann, I. Boustani, S.N. Rai, A.B. Alekseyev, G. Hirsch and R.J. Buenker, **Use of Relativistic Core Potentials to Compute Potential Curves and Lifetimes of Low-lying States of Arsenic Fluoride**, *Chem. Phys. Letters* **214**, 381-390 (1993).
- 290 A.B. Alekseyev, R.J. Buenker, H.-P. Liebermann and G. Hirsch, **Spin-orbit Configuration Interaction Study of the Potential Energy Curves and Radiative Lifetimes of the Low-lying States of Bismuth Hydride**, *J. Chem. Phys.* **100**, 2989-3001 (1994).
- 291 Y. Li, H.-P. Liebermann, G. Hirsch and R.J. Buenker, **Relativistic Configuration Interaction Study of the Electronic Spectrum of Thallium Chloride**, *J. Mol. Spectrosc.* **165**, 219-232 (1994).

- 292 M. Kimura, A. Dalgarno, L. Chantranupong, Y. Li, G. Hirsch and R.J. Buenker, **Nonradiative and Radiative Electron Capture in Collisions of He<sup>+</sup> Ions with C Atoms below 1000 eV**, *Phys. Rev. A* **49**, 2541-2544 (1994).
- 293 E. Leonardi, C. Petrongolo, V. Keshari, G. Hirsch and R.J. Buenker, ***Ab Initio* Study of NO<sub>2</sub>. Part IV. Vibrational Levels of the Ground Electronic State of N<sub>2</sub> in both the Diabatic and Adiabatic Representations of the Potential**, *Mol. Phys.* **82**, 553-565 (1994).
- 294 M. Kimura, J.P. Gu, Y. Li, G. Hirsch and R.J. Buenker, **Comment on ‘Suppressed Electron Capture in Slow O<sup>+</sup> (4S<sup>0</sup>, 2D<sup>0</sup>, 2P<sup>0</sup>)-He Collisions’**, *Phys. Rev. A* **49**, 3131-3133 (1994).
- 295 A.B. Alekseyev, H.-P. Liebermann, R.J. Buenker, G. Hirsch and Y. Li, ***Ab Initio Relativistic Configuration Interaction Calculations of the Spectrum of Bismuth Oxide: Potential Curves and Transition Probabilities***, *J. Chem. Phys.* **100**, 8956-8968 (1994).
- 296 J.P. Gu, R.J. Buenker and G. Hirsch, ***Ab Initio Study of the Electronic Spectrum of the Interstellar Free Radical CP***, *Chem. Phys.* **185**, 39-45 (1994).
- 297 M. Kimura, J.P. Gu, H.-P. Liebermann, Y. Li, G. Hirsch, R.J. Buenker and A. Dalgarno, **Electron Capture and Excitation in Collisions of O<sup>+</sup> (4S, 2D, 2P) Ions with He Atoms and He<sup>+</sup> Ions with O Atoms at Energies below 10 keV**, *Phys. Rev. A* **50**, 4854-4858 (1994).
- 298 P. Jensen, Y. Li, G. Hirsch, R.J. Buenker, T.J. Lee and I.N. Kozin, **Fourfold Clusters of Rovibrational Energies in H<sub>2</sub>Te Studied with an *Ab Initio* Potential Energy Function**, *Chem. Phys.* **190**, 179-189 (1995).
- 299 M. Kimura, J.P. Gu, G. Hirsch and R.J. Buenker, **Electron Capture in Collisions of N<sup>+</sup> (5S, 3P) with He: The Effect of Metastable Ions**, *Phys. Rev. A* **51**, 2063-2066 (1995).
- 300 J.P. Gu, G. Hirsch, R.J. Buenker, I.D. Petsalakis, G. Theodorakopoulos and M.B. Huang, **Electronic States and Radiative Transitions in LiAr**, *Chem. Phys. Letters* **230**, 473-479 (1994).
- 301 M. Dillon, M. Kimura, R.J. Buenker, G. Hirsch, Y. Li and L. Chantranupong, **Scattering Angle Dependence of Electron Impact Excitation: Intensity Variation within a Vibrational Progression**, *J. Chem. Phys.* **102**, 1561-1568 (1995).
- 302 A.B. Alekseyev, H.-P. Liebermann, R.J. Buenker and G. Hirsch, **Theoretical Study of the Electronic Spectrum of Antimony Oxide Employing Relativistic Effective Core Potentials**, *J. Chem. Phys.* **102**, 2539-2550 (1995).

- 303 K.K. Das, H.-P. Liebermann, R.J. Buenker and G. Hirsch, **Relativistic Configuration Interaction Study of the Low-lying Electronic States of Bi<sub>2</sub>**, *J. Chem. Phys.* **102**, 4518-4530 (1995).
- 304 M. Kolbuszewski, J.S. Wright and R.J. Buenker, **Avoided Crossings in Potential Curves of BF<sup>2+</sup>: A Study of Models for Bonding in Diatomic Dications**, *J. Chem. Phys.* **102**, 7519-7529 (1995).
- 305 J.P. Gu, R.J. Buenker, G. Hirsch and M. Kimura, **Potential Curves and Nonadiabatic Matrix Elements for Collisions Involving Fragments of the HeN<sup>+</sup> Molecular Ion**, *J. Chem. Phys.* **102**, 7540-7548 (1995).
- 306 A.B. Sannigrahi, R.J. Buenker and G. Hirsch, **Ab Initio Configuration Interaction Study of the Electronic Spectrum of SiH<sup>+</sup>**, *Chem. Phys. Letters* **237**, 204-211 (1995).
- 307 K.K. Das, H.-P. Liebermann, G. Hirsch and R.J. Buenker, **Use of Relativistic Effective Core Potentials in Calculating the Electronic Spectrum of the Antimony Dimer**, *J. Chem. Phys.* **102**, 8462-8473 (1995).
- 308 A.B. Alekseyev, A.B. Sannigrahi, H.-P. Liebermann, R.J. Buenker and G. Hirsch, **Ab Initio Potential Curves, Dipole Moments, and Transition Probabilities for the Low-lying States of Arsenic Oxide**, *J. Chem. Phys.* **103**, 234-244 (1995).
- 309 K.K. Das, A.B. Alekseyev, H.-P. Liebermann, G. Hirsch and R.J. Buenker, **Spin-orbit Configuration Interaction Study of the Electronic Spectrum of Antimony Iodide**, *Chem. Phys.* **196**, 395-406 (1995).
- 310 M. Kimura, Y. Li, G. Hirsch and R.J. Buenker, **Elastic and Inelastic Processes in H<sup>+</sup> + CH<sub>4</sub> Collisions in the Low-kilo-electron-volt Regime**, *Phys. Rev. A* **52**, 1196-1205 (1995).
- 311 A.B. Alekseyev, K.K. Das, H.-P. Liebermann, R.J. Buenker and G. Hirsch, **Ab Initio CI Study of the Electronic Spectrum of Bismuth Iodide Employing Relativistic Effective Core Potentials**, *Chem. Phys.* **198**, 333-344 (1995).
- 312 S. Krebs and R.J. Buenker, **A new Table-direct Configuration Interaction Method for the Evaluation of Hamiltonian Matrix Elements in a Basis of Linear Combinations of Spin-adapted Functions**, *J. Chem. Phys.* **103**, 5613-5629 (1995).
- 313 Z.-L. Cai, G. Hirsch and R.J. Buenker, **MRD-CI Study of the Electronic Spectrum of Na<sub>2</sub>Cl**, *Chem. Phys. Letters* **246**, 529-535 (1995).
- 314 A.V. Mitin, G. Hirsch and R.J. Buenker, **Accurate Atomic Gaussian Basis Functions for First-row Atoms I. Contracted Basis Sets Derived from 9s5p Primitives**, *J. Mol. Struct. THEOCHEM* **362**, 283-296 (1996).

- 315 A.B. Alekseyev, H.-P. Liebermann, R.J. Buenker and G. Hirsch, **Spin-orbit Configuration Interaction Study of the Potential Energy Curves and Transition Probabilities of the Mercury Hydride Molecule and Tests of Relativistic Effective Core Potentials for Hg, Hg<sup>+</sup> and Hg<sup>2+</sup>**, *J. Chem. Phys.* **104**, 4672-4684 (1996).
- 316 N. Shimakura, S. Suzuki, Y. Murakami, J.P. Gu, G. Hirsch, R.J. Buenker, M. Kimura and I. Shimamura, **Electron Capture and Target Excitation in Collisions of B<sup>q+</sup> and Be<sup>q+</sup> Ions with H and He Atoms at Energies below 10 keV/u**, *Phys. Scripta* **T62**, 39-42 (1996).
- 317 K.K. Das, H.-P. Liebermann, R.J. Buenker and G. Hirsch, **Ab Initio Configuration Interaction Calculations of the Potential Curves and Lifetimes of the Low-lying Electronic States of the Lead Dimer**, *J. Chem. Phys.* **104**, 6631-6642 (1996).
- 318 A.B. Alekseyev, H.-P. Liebermann, R.J. Buenker and G. Hirsch, **Ab Initio Study of the Low-lying States of SnH**, *Mol. Phys.* **88**, 591-603 (1996).
- 319 Z.-L. Cai, G. Hirsch and R.J. Buenker, **Ab Initio Study of the Electronic Spectrum of Na<sub>2</sub>F**, *Chem. Phys.* **207**, 43-49 (1996).
- 320 M. Kimura, J.P. Gu, G. Hirsch and R.J. Buenker, **Electron Capture in Collisions of O<sup>2+</sup>(<sup>3</sup>P) Ions with He Atoms at Energies below 10 keV: The Effect of Metastable O<sup>2+</sup>(<sup>1</sup>D) Ions**, *Phys. Rev. A* **53**, 4164-4168 (1996).
- 321 Z.-L. Cai, G. Hirsch and R.J. Buenker, **Ab Initio Study of the Electronic Spectrum of the PO<sub>2</sub> Radical**, *Chem. Phys. Letters* **255**, 350-356 (1996).
- 322 J.P. Gu, R.J. Buenker, G. Hirsch, P. Jensen and P.R. Bunker, **An Ab Initio Calculation of BH<sub>2</sub><sup>-</sup> Rovibronic Energies: A Very Small Singlet-Triplet Splitting**, *J. Mol. Spectrosc.* **178**, 172-183 (1996).
- 323 M. Kimura, A.B. Sannigrahi, J.P. Gu, G. Hirsch, R.J. Buenker and I. Shimamura, **Charge Transfer Rate in Collisions of H<sup>+</sup> Ions with Si Atoms**, *Astrophys. J.* **473**, 1114-1117 (1996).
- 324 M. Kimura, S. Suzuki, N. Shimakura, J.P. Gu, G. Hirsch, R.J. Buenker and I. Shimamura, **Charge Transfer in Collisions of B<sup>2+</sup> (<sup>2</sup>S, <sup>2</sup>P) and B<sup>3+</sup> (<sup>1</sup>S) Ions with He Atoms below 200 keV**, *Phys. Rev. A* **54**, 3029-3035 (1996).
- 325 M. Kimura, M.A. Dillon, R.J. Buenker, G. Hirsch, Y. Li and L. Chantranupong, **The Effect of Variable Electronic Transition Moment on the EELS Intensity Distribution within a Vibrational Progression: Use of the R-centroid Approximation to Analyze Results for the CO B-X and O<sub>2</sub> B'-X Transitions**, *Z. Phys. D* **38**, 165-169 (1996).
- 326 A.B. Alekseyev, H.-P. Liebermann, R.J. Buenker and G. Hirsch, **Theoretical Study of the Low-energy BiN Spectrum**, *Chem. Phys. Letters* **257**, 75-81 (1996).

- 327 A.V. Mitin, G. Hirsch and R.J. Buenker, **Accurate Small Split-valence 3-21SP and 4-22SP Basis Sets for the First-row Atoms**, *Chem. Phys. Letters* **259**, 151-158 (1996).
- 328 I.N. Kozin, P. Jensen, Y. Li, R.J. Buenker, G. Hirsch and S. Klee, **An *Ab Initio* Calculation of the Dipole Moment Surfaces and the Vibrational Transition Moments of the H<sub>2</sub>Te Molecule**, *J. Mol. Spectrosc.* **181**, 108-118 (1997).
- 329 E. Leonardi, C. Petrongolo, G. Hirsch and R.J. Buenker, ***Ab Initio* Study of NO<sub>2</sub>. V. Nonadiabatic Vibronic States and Levels of the  $\tilde{X}^2A_1/\tilde{A}^2B_2$  Conical Intersection**, *J. Chem. Phys.* **105**, 9051-9067 (1996).
- 330 M. Kimura, Y. Li, G. Hirsch and R.J. Buenker, **Elastic and Inelastic Processes in H<sup>+</sup>+C<sub>2</sub>H<sub>2</sub> Collisions below the 1.5-keV Regime**, *Phys. Rev. A* **54**, 5019-5026 (1996).
- 331 Y. Li, I.D. Petsalakis, H.-P. Liebermann, G. Hirsch and R.J. Buenker, ***Ab Initio* Configuration Interaction Calculations of the Predissociation of Rovibrational Levels of the C 3Π<sub>g</sub> and d 1Π<sub>g</sub> 3sσ Rydberg States of the Oxygen Molecule**, *J. Chem. Phys.* **106**, 1123-1133 (1997).
- 332 M. Kimura, J.P. Gu, G. Hirsch and R.J. Buenker, **Inelastic Processes in Collisions of H<sup>+</sup> Ions with C, N, O and Si Atoms below 1 keV**, *Phys. Rev. A* **55**, 2778-2785 (1997).
- 333 A.V. Mitin, G. Hirsch and R.J. Buenker, **Accurate Atomic Gaussian Basis Functions for Second-row Atoms. Small Split-valence 3-21SP and 4-22SP Basis Sets**, *J. Comput. Chem.* **18**, 1200-1210 (1997).
- 334 S. Krebs and R.J. Buenker, **Multireference Configuration Interaction Study of the Mixed Valence-Rydberg Character of the C<sub>2</sub>H<sub>4</sub> 1(π, π\*) V State**, *J. Chem. Phys.* **106**, 7208-7214 (1997).
- 335 J.S. Wright, D.J. Carpenter, A.B. Alekseyev, H.-P. Liebermann, R. Lingott and R.J. Buenker, **Thermodynamically Stable Diatomic Dications: Potential Curves and Radiative Lifetimes for CaCl<sup>2+</sup> Including Relativistic Effects**, *Chem. Phys. Letters* **266**, 391-396 (1997).
- 336 A.B. Alekseyev, H.-P. Liebermann, R. Lingott, R.J. Buenker and J.S. Wright, **Long-lived Diatomic Dications: Potential Curves and Radiative Lifetimes for CaBr<sup>2+</sup> and CaI<sup>2+</sup> Including Relativistic Effects**, *Mol. Phys.* **91**, 777-787 (1997).
- 337 P.C. Stancil, K. Kirby, A.B. Sannigrahi, R.J. Buenker, G. Hirsch and J.P. Gu, **The Photodissociation of SiH<sup>+</sup> in Interstellar Clouds and Stellar Atmospheres**, *Astrophys. J.* **486**, 574-579 (1997).
- 338 M. Kimura, J.P. Gu, G. Hirsch, R.J. Buenker, A. Domondon, T. Watanabe and H. Sato, **Electron Capture in Collisions of H<sup>+</sup> Ions with S Atoms and its Reverse Process below Kilo-electron-volt Energies**, *Phys. Rev. A* **56**, 1892-1896 (1997).

- 339 Y. Li, O. Bludský, G. Hirsch and R.J. Buenker, **Use of Gauss-Hermite Quadrature in the Treatment of Predissociation Resonances with the Complex-Scaling Method**, *J. Chem. Phys.* **107**, 3014-3020 (1997).
- 340 A.B. Alekseyev, H.-P. Liebermann, G. Hirsch and R.J. Buenker, **Relativistic Configuration Interaction Calculations of the Potential Curves and Radiative Lifetimes of the Low-lying States of Bismuth Nitride**, *Chem. Phys.* **225**, 247-258 (1997).
- 341 Y. Khandogin, A.B. Alekseyev, H.-P. Liebermann, G. Hirsch and R.J. Buenker, ***Ab Initio* Relativistic CI Calculations of the Spectroscopic Constants and Transition Probabilities for the Low-lying States of the BiOH/HBiO Isomers**, *J. Mol. Spectrosc.* **186**, 22-33 (1997).
- 342 I.D. Petsalakis, R.J. Buenker, G. Hirsch, and G. Theodorakopoulos, **Predissociation Widths and Lifetimes of the  $n = 3$   $^2\Sigma^+$  States of BeH and BeD**, *J. Phys. B: At. Mol. Opt. Phys.* **30**, 4935-4941 (1997).
- 343 A.B. Alekseyev, H.-P. Liebermann, G. Hirsch and R.J. Buenker, **The Spectrum of Arsenic Hydride: An *Ab Initio* Configuration Interaction Study Employing a Relativistic Effective Core Potential**, *J. Chem. Phys.* **108**, 2028-2040 (1998).
- 344 R.J. Buenker, A.B. Alekseyev, H.-P. Liebermann, R. Lingott and G. Hirsch, **Comparison of Spin-Orbit Configuration Interaction Methods Employing Relativistic Effective Core Potentials for the Calculation of Zero-field Splittings of Heavy Atoms with a  $^2\text{Po}$  Ground State**, *J. Chem. Phys.* **108**, 3400-3408 (1998).
- 345 P.C. Stancil, C.C. Havener, P.S. Krstić, D.R. Schultz, M. Kimura, J.P. Gu, G. Hirsch, R.J. Buenker and B. Zygelman, **Charge Transfer in Collisions of  $\text{C}^+$  with H and  $\text{H}^+$  with C**, *Astrophys. J.* **502**, 1006-1009 (1998).
- 346 J.P. Gu, G. Hirsch, R.J. Buenker, M. Kimura, C.M. Dutta and P. Nordlander, **Charge Transfer in Collisions of  $\text{C}^{2+}$  Ions with H Atoms at Low keV-Energies: A Possible Bound State of  $\text{CH}^{2+}$** , *Phys. Rev. A* **57**, 4483-4489 (1998).
- 347 I.D. Petsalakis, G. Theodorakopoulos, Y. Li, G. Hirsch, R.J. Buenker and M.S. Child, **Theoretical Study on the Rydberg States of NeH: *Ab Initio* Quantum Defect and Complex Coordinate Calculations**, *J. Chem. Phys.* **108**, 7607-7615 (1998).
- 348 A.B. Alekseyev, H.-P. Liebermann, R.M. Lingott, O. Bludský and R.J. Buenker, **The Spectrum of Antimony Hydride: An *Ab Initio* Configuration Interaction Study Employing a Relativistic Effective Core Potential**, *J. Chem. Phys.* **108**, 7695-7706 (1998).
- 349 Y. Li, G. Hirsch and R.J. Buenker, **Theoretical Treatment of Predissociation of the  $(4\text{p}\sigma)$   $^1,^3\Pi_u$  Rovibrational Levels in the Spectrum of the Oxygen Molecule**, *J. Chem. Phys.* **108**, 8123-8129 (1998).

- 350 P.C. Stancil, J.P. Gu, C.C. Havener, P.S. Krstić, D.R. Schultz, M. Kimura, B. Zygelman, G. Hirsch, R.J. Buenker and M.E. Bannister, **Electron Capture in Collisions of C<sup>+</sup> with H and H<sup>+</sup> with C**, *J. Phys. B: At. Mol. Opt. Phys.* **31**, 3647-3663 (1998).
- 351 O. Bludský, Y. Li, G. Hirsch and R.J. Buenker, **Comment on “On the direct complex scaling of matrix elements expressed in a discrete variable representation: Application to molecular resonances”**, *J. Chem. Phys.* **109**, 1201-1202 (1998).
- 352 R.J. Buenker, G. Hirsch and Y. Li, **Ab Initio Configuration Interaction Calculations of Rydberg and Mixed Valence-Rydberg States** in: *The Role of Rydberg States in Spectroscopy and Reactivity*, edited by C. Sándorfy (Kluwer, Dordrecht, 1999), pp. 57-91.
- 353 A.B. Alekseyev, H.-P. Liebermann, R.M. Lingott, R.J. Buenker, J.S. Wright, **Low-energy Spectrum of the Thermodynamically Stable BaI<sup>2+</sup> Dication**, *Spectrochim. Acta A* **55**, 467-475 (1999).
- 354 Y. Li, R.J. Buenker and G. Hirsch, **Theoretical Treatment of Predissociation of the CO (3sσ) B and (3pσ) C<sup>1Σ<sup>+</sup></sup> Rydberg States Based on a Rigorous Adiabatic Representation**, *Theor. Chem. Acc.* **100**, 112-116 (1998).
- 355 R.J. Buenker, Y. Li, G. Hirsch and M. Kimura, **Ab Initio Calculation of Proton-Hydrocarbon Scattering Cross Sections**, *J. Phys. Chem. A* **102**, 7127-7136 (1998).
- 356 R.J. Buenker and S. Krebs, **The Configuration-Driven Approach for Multireference Configuration Interaction Calculations**, in: *Recent Advances in Multireference Methods*, edited by K. Hirao (World Scientific, Singapore, 1999), pp. 1-29.
- 357 J.-P. Gu, G. Hirsch, R.J. Buenker, M. Kimura, C.M. Dutta and P. Nordlander, **Charge-Transfer Processes in Collisions of H<sup>+</sup> Ions with Phosphorus Atoms at Low Energies**, *Phys. Rev. A* **59**, 405-411 (1999).
- 358 R.J. Buenker, G. Hirsch, Y. Li, J.P. Gu, A.B. Alekseyev, H.-P. Liebermann and M. Kimura, **Ab initio Calculations of Excited Electronic State Potential Functions**, in: *Computational Molecular Spectroscopy*, edited by P. Jensen and P.R. Bunker (Wiley, West Sussex, 2000), pp. 135-168.
- 359 J.-P. Gu, G. Hirsch, R.J. Buenker, M. Brumm, G. Osmann, P.R. Bunker and P. Jensen, **A Theoretical Study of the Absorption Spectrum of Singlet CH<sub>2</sub>**, *J. Mol. Struct.* **517-518**, 247-264 (2000).
- 360 R.M. Lingott, H.-P. Liebermann, A.B. Alekseyev, and R.J. Buenker, **Electronic States and Transitions of Bismuth Sulfide**, *J. Chem. Phys.* **110**, 11294-11302 (1999).
- 361 J.S. Wright, G.A. DiLabio, D.R. Matusek, P.B. Corkum, M.Yu. Ivanov, C. Ellert, R.J. Buenker, A.B. Alekseyev and G. Hirsch, **Dissociation of Molecular Chlorine in a**

- Coulomb Explosion: Potential Curves, Bound States and Deviation from Coulombic Behavior for  $\text{Cl}_2^{n+}$  ( $n = 2, 3, 4, 6, 8, 10$ ), *Phys. Rev. A* **59**, 4512-4521 (1999).**
- 362 M. Honigmann, G. Hirsch, R.J. Buenker, I.D. Petsalakis and G. Theodorakopoulos, **Complex Coordinate Calculations on Autoionizing States of HeH and H<sub>2</sub>**, *Chem. Phys. Letters* **305**, 465-473 (1999).
- 363 I.D. Petsalakis, D. Papadopoulos, G. Theodorakopoulos and R.J. Buenker, **Theoretical Calculations on the Linewidths of Rovibrational Levels of the 3d Rydberg States of BeH and BeD**, *J. Phys. B: At. Mol. Opt. Phys.* **32**, 3225-3237 (1999).
- 364 G. Osmann, P.R. Bunker, P. Jensen, R.J. Buenker, J.-P. Gu and G. Hirsch, **A Theoretical Investigation of the Renner Interactions and Magnetic Dipole Transitions in the  $\tilde{A}$  -  $\tilde{X}$  Electronic Band System of HO<sub>2</sub>**, *J. Mol. Spectrosc.* **197**, 262-274 (1999).
- 365 S. Suzuki, N. Shimakura, J.-P. Gu, G. Hirsch, R.J. Buenker, M. Kimura and P.C. Stancil, **Electron Capture and Excitation in Collisions of Si<sup>2+</sup> Ions with He Atoms at Intermediate Energies**, *Phys. Rev. A* **60**, 4504-4509 (1999).
- 366 P.C. Stancil, D.R. Schultz, M. Kimura, J.-P. Gu, G. Hirsch and R.J. Buenker, **Charge Transfer in Collisions of O<sup>+</sup> with H and H<sup>+</sup> with O**, *Astron. Astrophys. Suppl. Series* **140**, 225-234 (1999).
- 367 Y. Li, O. Bludsky, G. Hirsch and R.J. Buenker, **Ab initio configuration interaction study of the predissociation of the (4s), (4pσ)  $^1,^3\Pi$  and (4pπ)  $^3\Sigma^+$  Rydberg states of HCl and DCl**, *J. Chem. Phys.* **112**, 260-267 (2000).
- 368 N. Balakrishnan, M.J. Jamieson, A. Dalgarno, Y. Li and R.J. Buenker, **Time-dependent quantum mechanical study of photodissociation of molecular oxygen in the Schumann-Runge continuum**, *J. Chem. Phys.* **112**, 1255-1259 (2000).
- 369 A.B. Alekseyev, H.-P. Liebermann, R.J. Buenker and D.B. Kokh, **Relativistic configuration interaction study of the ClF molecule and its emission spectra from 0<sup>+</sup> ion-pair states**, *J. Chem. Phys.* **112**, 2274-2284 (2000).
- 370 M. Kimura, J.-P. Gu, G. Hirsch, R.J. Buenker and P.C. Stancil, **Electron Capture in Collisions of Protons with CO Molecules in the keV Region: The Steric Effect**, *Phys. Rev. A* **61**, 1-9 (2000).
- 371 P.C. Stancil, K. Kirby, J.-P. Gu, G. Hirsch, R.J. Buenker and A.B. Sannigrahi, **The formation of SiH<sup>+</sup>, PH<sup>+</sup>, and SH<sup>+</sup> by radiative association**, *Astron. Astrophys. Suppl. Series* **142**, 107-112 (2000).
- 372 S. Roszak, M. Krauss, A.B. Alekseyev, H.-P. Liebermann and R.J. Buenker, **Spin-Orbit Configuration Interaction Calculation of the Potential Energy Curves of Iodine Oxide**, *J. Phys. Chem. A* **104**, 2999-3003 (2000).

- 373 R.J. Buenker and Y. Li, **On the Independence of Nonadiabatic Coupling Elements on the Choice of Origin of the Coordinate System**, *J. Chem. Phys.* **112**, 8318-8321 (2000).
- 374 R.J. Buenker, M. Honigmann, H.-P. Liebermann and M. Kimura, **Theoretical Study of the electronic structure of carbon dioxide: Bending potential curves and generalized oscillator strengths**, *J. Chem. Phys.* **113**, 1046-1054 (2000).
- 375 J.P. Gu, G. Hirsch, R.J. Buenker, M. Kimura, C.M. Dutta and P. Nordlander, **Charge Transfer in F<sup>2+</sup> Ions Colliding with He Atoms Below keV Energies and its Reverse Process**, *Phys. Rev. A* **62**, 052720, 1-7 (2000).
- 376 A.B. Alekseyev, H.-P. Liebermann, R.J. Buenker, N. Balakrishnan, H.R. Sadeghpour, S.T. Cornett and M.J. Cavagnero, **Spin-orbit effects in photodissociation of sodium iodide**, *J. Chem. Phys.* **113**, 1514-1523 (2000).
- 377 J.M. Brown, R.J. Buenker, A. Carrington, C. diLauro, R.N. Dixon, R.W. Field, J.T. Hougen, W. Hüttner, K. Kuchitsu, A.J. Merer, T.A. Miller, M. Quack, D.A. Ramsay, A.J. Stone, L. Veseth, R.N. Zare, **Remarks on the signs of g-factors in atomic and molecular Zeeman spectroscopy**, in *Mol. Phys.* **98**, 1597-1601 (2000).
- 378 T. Kusakabe, K. Asahina, J.P. Gu, G. Hirsch, R.J. Buenker, M. Kimura, H. Tawara and Y. Nakai, **Charge-transfer processes in collisions of H<sup>+</sup> ions with H<sub>2</sub>, D<sub>2</sub>, CO, and CO<sub>2</sub> molecules in the energy range 0.2 – 4.0 keV**, *Phys. Rev. A* **62**, 062714, 1-7 (2000).
- 379 T. Kusakabe, K. Asahina, A. Iida, Y. Tanaka, J.P. Gu, G. Hirsch, R.J. Buenker, M. Kimura, H. Tawara and Y. Nakai, **Charge-transfer processes in collisions of slow H<sup>+</sup> ions with hydrocarbon molecules: CH<sub>4</sub>, C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>6</sub>, and C<sub>3</sub>H<sub>8</sub>**, accepted for publication in *Phys. Rev. A* **62**, 062715, 1-6 (2000).
- 380 I.D. Petsalakis, R.J. Buenker, H.-P. Liebermann, A.B. Alekseyev, A.Z. Devdariani and G. Theodorakopoulos, **Potential energy curves and dipole transition moments to the ground state of the system Ar\*(3p<sup>5</sup>4s, <sup>3</sup>P, <sup>1</sup>P) + Ne**, *J. Chem. Phys.* **113**, 5812-5816 (2000).
- 381 A.B. Alekseyev, H.-P. Liebermann, D.B. Kokh and R.J. Buenker, **On the ultraviolet photofragmentation of hydrogen iodide**, *J. Chem. Phys.* **113**, 6174-6185 (2000).
- 382 K.D. Setzer, C. Uibel, W. Zymicki, A.M. Pravilov, E.H. Fink, H.-P. Liebermann, A.B. Alekseyev and R.J. Buenker, **Experimental and Theoretical Study of the Electronic States and Spectra of BiNa**, *J. Mol. Spectrosc.* **204**, 163-175 (2000).
- 383 R. Suzuki, A. Watanabe, H. Sato, J.P. Gu, G. Hirsch, R.J. Buenker, M. Kimura and P.C. Stancil, **Electron-Capture Dynamics in Collisions of Si<sup>4+</sup> Ions with He Atoms at Intermediate Energies**, *Phys. Rev. A* **63**, 042717, 1-5 (2001).

- 384 A.V. Titov, N.S. Mosyagin, A.B. Alekseyev and R.J. Buenker, **GRECP/MRD-CI calculations of spin-orbit splitting in ground state of Tl and of spectroscopic properties of TiH**, *Int. J. Quant. Chem.* **81**, 409-421 (2001).
- 385 P. Jensen, R.J. Buenker, J.-P. Gu, G. Osmann and P.R. Bunker, **Refined potential-energy surfaces for the  $\tilde{X}^2A''$  and  $\tilde{A}^2A'$  electronic states of the HO<sub>2</sub> molecule**, *Can. J. Phys.* **79**, 641-652 (2001).
- 386 R.J. Buenker, H.-P. Liebermann and J.L. Whitten, **Excited electronic states of CO adsorbed on platinum**, *Chem. Phys.* **265**, 1-11 (2001).
- 387 D.B. Kokh, Y. Li, R.J. Buenker, A.B. Alekseyev and H.-P. Liebermann, **Nonadiabatic effects in the lowest  $0^+(^3P)$  ion-pair states of ClF**, *J. Chem. Phys.* **114**, 3003-3009 (2001).
- 388 K.D. Setzer, E.H. Fink, A.B. Alekseyev, H.-P. Liebermann and R.J. Buenker, **Experimental and Theoretical Study of the Electronic States and Spectra of TeH and TeLi**, *J. Mol. Spectrosc.* **206**, 181-197 (2001).
- 389 V. Rai., H.-P. Liebermann, A.B. Alekseyev and R.J. Buenker, **Electronic states and transitions of tellurium fluoride**, *J. Chem. Phys.* **114**, 8386-8394 (2001).
- 390 A. Watanabe, H. Sato, J.P. Gu, G. Hirsch, R.J. Buenker and M. Kimura, **Electron capture in collisions of Al<sup>2+</sup> ions with He atoms at intermediate energies**, *Phys. Rev. A* **64**, 032717, 1-7 (2001).
- 391 A. Z. Devdariani, A.L. Zagrebin, M.G. Lednev, A.B. Alekseyev, H.-P. Liebermann and R.J. Buenker, **Hg\* + He at moderate interatomic separations and radiative decay of the Hg(6<sup>3</sup>P<sub>2</sub>) metastable state in collisions with He atoms**, *Opt. and Spectrosc.* **91**, 833-841 (2001).
- 392 Y. Li, H.-P. Liebermann and R.J. Buenker, **Ab initio calculation of predissociation linewidths in the Schumann-Runge bands of the oxygen molecule**, *J. Chem. Phys.* **114**, 10396-10401 (2001).
- 393 N. Balakrishnan, A.B. Alekseyev and R.J. Buenker, **Ab initio quantum mechanical investigation of the photodissociation of HI and DI**, *Chem. Phys. Letters.* **341**, 594-600 (2001).
- 394 M. Tachikawa, I. Shimamura, R.J. Buenker and M. Kimura, **Bound States of Positron with Molecules**, in: *New Directions in Antimatter Chemistry and Physics*, C.M. Surko and F.A. Gianturco (eds.), Kluwer Academic Publ., 2001, pp. 437-450.
- 395 S.N. Yurchenko, P. Jensen, Yan Li, R.J. Buenker and P.R. Bunker, **The Near Ultraviolet Band System of Singlet Methylene**, *J. Mol. Spectrosc.* **208**, 136-143 (2001).

- 396 I. Boustani, R. Buenker, V.N. Shrednik, M.V. Loginov, M.M. Korsukova and V.N. Gurin, **Formation and stability of free charged lanthanum hexaboride clusters at field evaporation**, *J. Chem. Phys.* **115**, 3297-3307 (2001).
- 397 I.D. Petsalakis, G. Theodorakopoulos, H.-P. Liebermann and R.J. Buenker, **Potential energy curves and dipole transition moments for electronic states of ArHe and HeNe**, *J. Chem. Phys.* **115**, 6365-6372 (2001).
- 398 T. Kusakabe, R.J. Buenker and M. Kimura, **Charge Transfer Processes in Collisions of H<sup>+</sup> Ions with H<sub>2</sub>, D<sub>2</sub>, CO, CO<sub>2</sub>, CH<sub>4</sub>, C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>6</sub> and C<sub>3</sub>H<sub>8</sub> Molecules Below 10 keV**, *Atomic and Plasma-Material Interaction Data for Fusion (IAEA)*, Vol. 10, pp. 151-161 (2002).
- 399 D.B. Kokh, A.B. Alekseyev and R.J. Buenker, **Ab initio study of spectroscopic and radiative characteristics of ion-pair states of the Cl<sub>2</sub> molecule**, *J. Chem. Phys.* **115**, 9298-9310 (2001).
- 400 R. Suzuki, A. Watanabe, H. Sato, J.P. Gu, G. Hirsch, R.J. Buenker, M. Kimura and P.C. Stancil, **Charge Transfer Processes in Collisions of Si<sup>4+</sup> Ions with He Atoms at Intermediate Energies**, *Phys. Scripta* **T92**, 345-347 (2001).
- 401 V. Rai, H.-P. Liebermann, R.J. Buenker, A.B. Alekseyev and R. Zellner, **Electronic states and transitions of the TeX (X = Cl, Br, I) radicals**, *Mol. Phys.* **100**, 809-820 (2001).
- 402 K.K. Das, I.D. Petsalakis, H.-P. Liebermann, A.B. Alekseyev and R.J. Buenker, **Ab initio spin-orbit CI calculations of the potential curves and radiative lifetimes of low-lying states of lead monofluoride**, *J. Chem. Phys.* **116**, 608-616 (2002).
- 403 M.A. Green, P.J.O. Teubner, L. Campbell, M.J. Brunger, M. Hoshino, T. Ishikawa, M. Kitajima, H. Tanaka, Y. Itikawa, M. Kimura and R.J. Buenker, **Absolute Differential Cross Sections for Electron Impact Excitation of the 10.8 – 11.5 eV Energy-Loss States of CO<sub>2</sub>**, *J. Phys. B: At. Mol. Opt. Phys.* **35**, 567-587 (2002).
- 404 I.D. Petsalakis, G. Theodorakopoulos and R.J. Buenker, **Complex coordinate calculations on predissociation states of diatomic molecules**, *Russ. J. Phys. Chem.* **76**, Supplement 1, 1-6 (2002).
- 405 R.J. Buenker, **Dynamical Aspects of Longitudinal Polarization Measurements for Weak Decay Processes: Suggestion for an Experimental Test of the Two-Component Theory of the Neutrino**, *Russ. J. Phys. Chem.* **76**, Supplement 1, 144-156 (2002).
- 406 N.S. Mosyagin, A.V. Titov, R.J. Buenker, H.-P. Liebermann and A.B. Alekseyev, **GRECP/MRD-CI calculations on the Hg atom and the HgH molecule**, *Int. J. Quantum Chem.* **88**, 681-686 (2002).

- 407 T.A. Isaev, N.S. Mosyagin, A.V. Titov, A.B. Alekseyev and R.J. Buenker, **GRECP/5e-MRD-CI calculation of the electronic structure of PbH**, *Int. J. Quantum Chem.* **88**, 687-690 (2002).
- 408 R.J. Buenker, **Use of Hamilton's canonical equations to modify Newton's corpuscular theory of light: A missed opportunity**, *Khim. Fyz.* **22** (10), 124-128 (2003); see also <http://arxiv.org/physics/0411110>.
- 409 R.J. Buenker and P.L. Muiño, **Quantum Mechanical Relations for the Energy, Momentum and Velocity of Single Photons in Dispersive Media**, *Khim. Fyz.* **23** (2), 111-116 (2004); see also <http://arxiv.org/physics/0607094>.
- 410 P.L. Muiño, A.M. Thompson and R.J. Buenker, **Use of time-correlated single photon counting detection to measure the speed of light in water**, *Khim. Fyz.* **23** (2), 117-128 (2004); see also <http://arxiv.org/physics/0502100>.
- 411 R.J. Buenker, J.L. Whitten, E.I. Izgorodina, H.-P. Liebermann and D.B. Kokh, **Use of exchange maximization to generate starting vectors for self-consistent field calculations on metal cluster/adsorbate systems**, *J. Comput. Chem.* **23**, 943-949 (2002).
- 412 D.B. Kokh, A.B. Alekseyev, Yan Li, R.J. Buenker, **The lowest  $1(^3\text{P}_J)$  and  $2(^3\text{P}_2)$  ion-pair states of ClF: nonadiabatic effects and emission spectra**, *J. Chem. Phys.* **117**, 628-635 (2002).
- 413 G. V. Golubkov, M. G. Golubkov and R.J. Buenker, **Dissociative recombination of slow electrons with molecular oxygen ions in the intense laser field**, *Khim. Fyz.* **23** (2), 53-60 (2004).
- 414 A.Z. Devdariani and R.J. Buenker, **He ( $2^1,3^3\text{S}$ ) Quasimolecule at Low Temperatures**, *Khim. Fyz.* **23** (2), 61-64 (2004).
- 415 I.D. Petsalakis, G. Theodorakopoulos, H.-P. Liebermann and R.J. Buenker, **Potential energy curves and dipole transition moments for excited electronic states of XeKr and ArNe**, *J. Chem. Phys.* **117**, 3639-3646 (2002)
- 416 G. Theodorakopoulos, I.D. Petsalakis, H.-P. Liebermann, R.J. Buenker and J. Koput, **Ab initio calculations on electronic states of CaOH**, *J. Chem. Phys.* **117**, 4810-4819 (2002).
- 417 D. Giri, R.J. Buenker and K.K. Das, **Electronic Spectrum of Tin Oxide: MRDCI Study**, *J. Phys. Chem. A.* **106**, 8790-8797 (2002).
- 418 K.D. Setzer, J. Borkowska-Burnecka, W. Zyrnicki, A.M. Pravilov, E.H. Fink, K.K. Das, H.-P. Liebermann, A.B. Alekseyev and R.J. Buenker, **Experimental and Theoretical Study of the Electronic States and Spectra of PbLi**, *J. Mol. Spectrosc.* **217**, 127-141 (2003).

- 419 P.G. Alcheev, R.J. Buenker, V.E. Chernov and B.A. Zon, **Oscillator strengths for Rydberg states in ArH calculated in QDT approximation**, *J. Mol. Spectrosc.* **218**, 190-196 (2003).
- 420 L. Pichl, Y. Li, H.-P. Liebermann, R.J. Buenker and M. Kimura, **Charge transfer for the ground state O<sup>+</sup> (4S) ion in collision with H<sub>2</sub> molecules**, *J. Chem. Phys.* **118**, 4872-4877 (2003).
- 421 R.J. Buenker, **The Lorentz Transformation Sign Ambiguity and Its Relation to Measured Faster-than-c Photon Speeds**, *Khim. Fyz.* **23** (7), 80-82 (2004); see also <http://arxiv.org/physics/0411109>.
- 422 A.B. Alekseyev, H.-P. Liebermann and R.J. Buenker, **Spin-orbit Multireference Configuration Iteration Method and Applications to Systems Containing Heavy Atoms**, in: *Relativistic Molecular Calculations*, edited by K. Hirao and M. Ishikawa (World Scientific, Singapore, 2003), pp. 65-105.
- 423 S.N. Rai, H.-P. Liebermann, R.J. Buenker and M. Kimura, **Ab initio CI calculations of the potential curves and nonadiabatic coupling matrix elements for collisions of protons with the ethylene molecule**, *Int. J. Quantum Chem.* **95**, 866-876 (2003).
- 424 R.J. Buenker, H.-P. Liebermann, D. B. Kokh, E.I. Izgorodina and J.L. Whitten, **Configuration Interaction Study of the Excited States of CO Adsorbed on a Pt<sub>97</sub> Cluster**, *Chem. Phys.* **291**, 115-124 (2003).
- 425 T.W. Imai, M. Kimura, J.P. Gu, G. Hirsch, R.J. Buenker, J.G. Wang, P.C. Stancil and L. Pichl, **Ab initio study of one- and two-electron transfer processes in collisions of Ne<sup>2+</sup> with He at low to intermediate energies**, *Phys. Rev. A* **68**, 012716, 1-7 (2003).
- 426 G.V. Golubkov, M.G. Golubkov, A.N. Romanov and R.J. Buenker, **Dissociative Recombination e<sup>-</sup> + O<sub>2</sub><sup>+</sup> → O(1D) + O(3P) in a strong laser field**, *Phys. Chem. Chem. Phys.* **5**, 3174-3182 (2003).
- 427 L. Pichl, Y. Li, R.J. Buenker and M. Kimura, **Electron capture and excitation in collisions of O<sup>+</sup> (4S, 2D, 2P) with H<sub>2</sub> molecules**, *Phys. Rev. A* **69**, 062715, 1-10 (2004).
- 428 I.D. Petsalakis, G. Theodorakopoulos and R.J. Buenker, **Theoretical ab initio study of the electronic states of KrH and KrH<sup>+</sup>. Quantum defect and complex coordinate calculations on the Rydberg states of KrH**, *J. Chem. Phys.* **119**, 2004-2013 (2003).
- 429 M. Tachikawa, R.J. Buenker and M. Kimura, **Bound states of positron with urea and acetone molecules using configuration interaction ab initio molecular orbital approach**, *J. Chem. Phys.* **119**, 5005-5009 (2003).
- 430 A.J. Yencha, P. Baltzer, A.J. Cormack, Y. Li, H.-P. Liebermann, A.B. Alekseyev and R.J. Buenker, **High-resolution photoelectron spectroscopy of HI and DI: Experimental and theoretical analysis of the A 2Σ<sup>+</sup> ion system**, *J. Chem. Phys.* **119**, 5943-5948 (2003).

- 431 T. Kusakabe, M. Kimura, L. Pichl, R.J. Buenker and H. Tawara, **Observation of significant differences in charge transfer between collisions of  $H^+$  ions with  $H_2$  and with  $D_2$  molecules in the high-eV to low-KeV range**, *Phys. Rev. A* **68**, 050701(R), 1-4 (2003).
- 432 L. Pichl, R.J. Buenker and M. Kimura, **Calculation of Cross Sections for Proton and Antiproton Stopping in Molecules**, *Adv. Quant. Chem.* **46**, 165-193 (2004).
- 433 R.M. Lingott, H.-P. Liebermann, A.B. Alekseyev and R.J. Buenker, *Ab initio study of the BiSe and BiTe electronic spectra: What happens with  $X_2-X_1$  emission in the heavier Bi chalcogenides?*, *J. Chem. Phys.* **120**, 7476-7482 (2004).
- 434 S. Wu, Y. Chen, X. Yang, Y. Guo, Y. Li, R.J. Buenker and P. Jensen, **Vibronic transition moments and line intensities for  $H_2O^+$** , *J. Mol. Spectrosc.* **225**, 96-106 (2004).
- 435 Y. Li, H.-P. Liebermann, R.J. Buenker and L. Pichl, **A coupled treatment of  $1\Sigma^+$  and  $3\Pi$  states of AgH molecule**, *Chem. Phys. Letters* **389**, 101-107 (2004).
- 436 D.B. Kokh, A.B. Alekseyev and R.J. Buenker, **Theoretical study of the UV absorption in  $Cl_2$ : Potentials, transition moments, extinction coefficients, and  $Cl^*/Cl$  branching ratio**, *J. Chem. Phys.* **120**, 11549-11556 (2004).
- 437 R.J. Buenker, **Comparison of the phenomena of light refraction and gravitational bending**, *Khim. Fys.* **24** (4), 29-35 (2005); see also <http://arxiv.org/abs/0904.3232>.
- 438 R.J. Buenker, **The Lorentz Transformation for photons in dispersive media**, *Khim. Fys.* **24** (9), 19-24 (2005); see also <http://arxiv.org/abs/physics/0606172>.
- 439 L. Pichl, M. Kimura, Y. Li and R.J. Buenker, **Branching ratios for secondary processes of water ions induced by proton beams in radiation therapy of cancer**, *IEEE Trans. Nucl. Sci.* **51**, 1481-1484 (2004).
- 440 H. Suno, S.N. Rai, H.-P. Liebermann, R.J. Buenker, M. Kimura and R.K. Janev, **Elastic and inelastic processes in  $H^+ + CH_2$  collisions between 0.5 and 1.5 keV**, *Phys. Rev. A* **70**, 032703, 1-7 (2004).
- 441 L. B. Zhao, P.C. Stancil, J.P. Gu, H.-P. Liebermann, Y. Li, P. Funke, R.J. Buenker, B. Zygelman, M. Kimura and A. Dalgarno, **Radiative charge transfer in collisions of O with  $He^+$** , *Ap. J.* **615**, 1063-1072 (2004).
- 442 M. Tachikawa, R.J. Buenker and M. Kimura, **Geometry relaxation effects for molecules as a result of binding with a positron**, *J. Chem. Phys.* **121**, 9191-9192 (2004).
- 443 T. Kusakabe, L. Pichl, R. J. Buenker, M. Kimura and H. Tawara, **Isotope effect in charge transfer collisions of slow  $H^+$  and  $D^+$  ions with  $H_2$ ,  $HD$ , and  $D_2$  molecules**, *Phys. Rev. A* **70**, 052710, 1-7 (2004).

- 444 D. Dai, M.-H. Whangbo, A. Ugrinov, S.C. Sevov, F. Wang, L. Li, A. Villesuzanne, A. B. Alekseyev, H.-P. Liebermann and R.J. Buenker, **Analysis of the effect of spin-orbit coupling on the electronic structure of the Bi<sub>2</sub><sup>2-</sup> anion in (K-crypt)<sub>2</sub>Bi<sub>2</sub> on the basis of relativistic electronic structure calculations**, *J. Phys. Chem. A* **109**, 1675-1683 (2005).
- 445 R. Suzuki, S. N. Rai, H.-P. Liebermann, R. J. Buenker, L. Pichl and M. Kimura, **Elastic and electron-capture processes in H<sup>+</sup> + C<sub>2</sub>H<sub>4</sub> collisions below the 10-keV regime**, *Phys. Rev. A* **71**, 032710, 1-10 (2005).
- 446 A. B. Alekseyev, D. B. Kokh and R. J. Buenker, **HI photofragmentation revisited. Comment on “Probing excited electronic states using vibrationally mediated photolysis: Application to hydrogen iodide,”** *J. Phys. Chem. A* **109**, 3094-3096 (2005).
- 447 R. J. Buenker, H.-P. Liebermann, V. Melnikov, M. Tachikawa, L. Pichl and M. Kimura, **Positron binding energies for alkali hydrides**, *J. Phys. Chem. A* **109**, 5956-5964 (2005).
- 448 L. B. Zhao, P.C. Stancil, H.-P. Liebermann, P. Funke and R.J. Buenker, **Charge transfer between O+ ions and helium**, *Phys. Rev. A* **71**, 060701 (R), 1-4 (2005).
- 449 C. Y. Lin, P. C. Stancil, J. P. Gu, R. J. Buenker and M. Kimura, **Electron capture in collisions of N<sup>+</sup> with H and H<sup>+</sup> with N**, *Phys. Rev. A* **71**, 062708, 1-7 (2005).
- 450 L. Pichl, M. Tachikawa, R. J. Buenker, M. Kimura and J.-M. Rost, **The effects of positron binding and annihilation mechanisms in biomolecules on PET resolution**, *IEEE Trans. Nucl. Sci.* **52**, 2810-2817 (2005).
- 451 L. B. Zhao, P. C. Stancil, J. P. Gu, H.-P. Liebermann, P. Funke, R. J. Buenker and M. Kimura, **Electron capture in collisions of S with H<sup>+</sup>**, *Phys. Rev. A* **71**, 062713, 1-11 (2005).
- 452 L. Pichl, Y. Li, R. J. Buenker, M. Kimura, J. Horacek and I. Schneider, **Electronic potential energy of H<sub>2</sub><sup>-</sup> and CHe<sup>4+</sup> diatomic ions**, *J. Plasma Fusion Research SERIES 7*, 249-252 (2006).
- 453 V. Rai-Constapel, H.-P. Liebermann, R. J. Buenker and S. N. Rai, **Ab initio MRD-CI study of the spectrum of the TeO molecule employing relativistic effective core potentials**, *J. Phys. Chem. A* **110**, 404-411 (2006).
- 454 D.B. Kokh, R. J. Buenker, H.-P. Liebermann, L. Pichl and J. L. Whitten, **Theoretical study of the CH<sub>2</sub> + O photodissociation of formaldehyde adsorbed on the Ag (111) surface**, *J. Phys. Chem. B* **109**, 18070-18080 (2005).
- 455 L. B. Zhao, P. C. Stancil, J.-P. Gu, G. Hirsch, R. J. Buenker, T. W. Imai and M. Kimura, **Charge transfer between S<sup>2+</sup> and He: A comparative study of quantal and semiclassical approaches**, *Phys. Rev. A* **72**, 032719, 1-9 (2005).

- 456 R. Suzuki, S. N. Rai, H.-P. Liebermann, R. J. Buenker, L. Pichl and M. Kimura, **Elastic and inelastic processes in  $H^+ + C_2H_6$  collisions below the 10-keV regime**, *Phys. Rev. A* **72**, 052710, 1-10 (2005).
- 457 C. M. Dutta, J.-P. Gu, G. Hirsch, R. J. Buenker, P. Nordlander and M. Kimura, **Charge-transfer processes in  $F^{2+} + H \rightarrow F^+ + H^+$  collisions and the reverse process at low keV energies**, *Phys. Rev. A* **72**, 052715, 1-7 (2005).
- 458 L. Pichl, R. Suzuki, M. Kimura, Y. Li, R. J. Buenker, M. Hoshino and Y. Yamazaki, **Angular dependence of double electron capture in collisions of  $C^{4+}$  with He. Stueckelberg oscillations in the differential cross-section for capture into  $C^{2+}$  ( $1s^22s^2$   
 $^1S$ )**, *Eur. Phys. J. D* **38**, 59-64 (2006).
- 459 R.J. Buenker, H.-P. Liebermann, M. Tachikawa, L. Pichl and M. Kimura, **Multireference CI study of the potential curves and properties of positronic complexes of alkali hydrides**, *Nucl. Instr. and Meth. in Phys. Res. B* **247**, 47-51(2006).
- 460 F. A. Gianturco, J. Franz, R. J. Buenker, H.-P. Liebermann, L. Pichl, J.-M. Rost, M. Tachikawa and M. Kimura, **Positron binding to alkali hydrides: the role of molecular vibrations**, *Phys. Rev. A* **73**, 022705, 1-9 (2006).
- 461 M. Kimura, L. Pichl, Y. Li, H.-P. Liebermann, R. J. Buenker and I. F. Schneider, **Steric effect in  $O^+/H_2$  and  $H^+/H_2O$  collisions. Charge transfer in  $H_2O^+$  and  $H_3O^+$  collision intermediate systems**, *Eur. Phys. J. D* **38**, 85-91 (2006).
- 462 H. Suno, S. N. Rai, H.-P. Liebermann, R. J. Buenker, M. Kimura and L. Pichl, **Elastic and inelastic processes in  $H^+ + NH_2$  collisions between 0.5 and 1.5 keV**, *Phys. Rev. A* **74**, 012701, 1-7 (2006).
- 463 A. Devdariani, E. Chesnokov, A. Zagrebin, M. G. Lednev, I. D. Petsalakis, G. Theodorakopoulos, H.-P. Liebermann and R. J. Buenker, **Quasi-molecular radiative transitions produced by thermal and low-temperature collisions: Ar ( $3p^6$   $^1S_0$ - $3p^54s^3P_2$ )-He**, *Chem. Phys.* **330**, 101-112 (2006).
- 464 D. B. Kokh, R. J. Buenker and J. L. Whitten, **Trends in adsorption of open-shell atoms and small molecular fragments on the Ag (111) surface**, *Surf. Sci.* **600**, 5104-5113 (2006).
- 465 M. Honigmann, R. J. Buenker and H.-P. Liebermann, **Complex SCF and MRD-CI calculations for the  $^2\Pi_g$  resonance state of  $N_2^-$** , *J. Chem. Phys.* **125**, 234304, 1-12 (2006)
- 466 L. B. Zhao, J. G. Wang, P. C. Stancil, J.-P. Gu, H.-P. Liebermann, R. J. Buenker and M. Kimura, **Radiative charge transfer in  $Ne^{2+} + He$  collisions**, *J. Phys. B: At. Mol. Opt. Phys.* **39**, 5151-5160 (2006).
- 467 M. Hoshino, L. Pichl, Y. Kanai, Y. Nakai, M. Kitajima, M. Kimura, Y. Li, H.-P. Liebermann, R. J. Buenker, H. Tanaka and Y. Yamazaki, **Experimental and theoretical**

- study of double-electron capture in collisions of slow C<sup>4+</sup> (1s<sup>2</sup> 1S) with He (1s<sup>2</sup> 1S), *Phys. Rev. A.* **75**, 012716, 1-6 (2007).
- 468 R. J. Buenker, H.-P. Liebermann and A. Z. Devdariani, **Ab initio spin-orbit configuration interaction calculations for high-lying states of the HeNe quasi-molecule**, *J. Phys. Chem. A* **111**, 1307-1318 (2007).
- 469 S. Mada, K. Hida, M. Kimura, L. Pichl, H.-P. Liebermann, Y. Li and R. J. Buenker, **Charge transfer and electronic excitation on collisions of protons with water molecules below 10 eV**, *Phys. Rev. A* **75**, 022706, 1-7 (2007).
- 470 R. J. Buenker, H-P. Liebermann, L. Pichl, M. Tachikawa and M. Kimura, **Role of the electric dipole moment in positron binding to the ground and excited states of the BeO molecule**, *J. Chem. Phys.* **126**, 104305, 1-7 (2007).
- 471 G. J. Vazquez, J. M. Amero, H.-P. Liebermann, R. J. Buenker and H. Lefebvre-Brion, **An insight into the lowest Rydberg states of CH**, *J. Chem. Phys.* **126**, 164302, 1-13 (2007).
- 472 T. Kusakabe, H. Tawara, M. Kimura, J.-P. Gu and R. J. Buenker, **Charge-transfer cross sections of H<sup>+</sup> ions in collisions with Ne atoms in the energy range below 4.0 keV**, *Phys. Rev. A* **75**, 044701, 1-3 (2007).
- 473 A. B. Alekseyev, H.-P. Liebermann and R. J. Buenker, **An ab initio study of the CH<sub>3</sub>I photodissociation. I. Potential energy surfaces**, *J. Chem. Phys.* **126**, 234102, 1-11 (2007).
- 474 A. B. Alekseyev, H.-P. Liebermann and R. J. Buenker, **An ab initio study of the CH<sub>3</sub>I photodissociation. II. Transition moments, absorption spectra, I\* quantum yields**, *J. Chem. Phys.* **126**, 234103, 1-11 (2007).
- 475 C. Y. Lin, P. C. Stancil, Y. Li, J.-P. Gu, H.-P. Liebermann, R. J. Buenker and M. Kimura, **Vibrationally-resolved charge transfer for proton collisions with CO and H collisions with CO<sup>+</sup>**, *Phys. Rev. A* **76**, 012702, 1-9 (2007).
- 476 D. B. Kokh, R. J. Buenker, H.-P. Liebermann, and J. L. Whitten, **Theoretical study of the photo-induced C-H bond cleavage in formaldehyde adsorbed on the Ag(111) surface**, *J. Phys. Chem. C* **111**, 9914-9918 (2007).
- 477 V. Rai-Constapel, H.-P. Liebermann, R. J. Buenker, M. Honigmann and P. Jensen, **A theoretical study of TeOH in its electronic ground state**, *J. Mol. Spectrosc.* **244**, 102-108 (2007).
- 478 A. B. Alekseyev, H.-P. Liebermann, and R. J. Buenker, **Theoretical study of the ArH+ photodissociation**, *Phys. Chem. Chem. Phys.* **9**, 5088-5095 (2007).
- 479 T. Kusakabe, K. Gotanda, M. Kimura, S. N. Rai, H.-P. Liebermann, and R. J. Buenker, **Vibrational temperature effect on charge-transfer processes in collisions of H<sup>+</sup> and O<sup>+</sup>**

- ions with C<sub>2</sub>H<sub>4</sub> molecules at energies below 10 keV/u, *Phys. Rev. A.* **76**, 042711, 1-7 (2007).**
- 480 R. J. Buenker and H.-P. Liebermann, **Configuration interaction calculations of positron binding to molecular oxides and hydrides and its effect on spectroscopic constants, *Nucl. Instr. and Meth. in Phys. Res. B* **266**, 483-490 (2008).**
- 481 R. J. Buenker, **The global positioning system and the Lorentz transformation, *Apeiron* **15**, 254-269 (2008).**
- 482 R. J. Buenker, **Huygens' principle and computation of the light trajectory responsible for the gravitational displacement of star images, *Apeiron* **15**, 338-357 (2008).**
- 483 A. B. Alekseyev, R. J. Buenker and H.-P. Liebermann, **Ab initio study of the KrH<sup>+</sup> photodissociation, *J. Chem. Phys.* **128**, 234308, 1-7 (2008).**
- 484 S. Fukata, M. Kimura, Y. Li, H.-P. Liebermann, R. J. Buenker and L. Pichl, **Comparison of charge transfer in proton collisions with methane and silane for simulations of cold plasma, *Plasma and Fusion Research* **3**, S1040, 1-3 (2008).**
- 485 M. V. Khoma, M. Imai, O. M. Karbovanets, Y. Kikuchi, M. Saito, Y. Haruyama, M. I. Karbovanets, I. Yu. Kretinin, A. Itoh and R. J. Buenker, **A simple theoretical approach of charge transfer processes in collisions of atomic ions with polar targets, *Chem. Phys.* **352**, 142-146 (2008).**
- 486 A. B. Alekseyev, H.-P. Liebermann and R. J. Buenker, **Spin-orbit configuration interaction study of the ultraviolet photofragmentation of XeH<sup>+</sup>, *Phys. Chem. Chem. Phys.* **10**, 5706-5713 (2008).**
- 487 M. Nagao, K. Hida, M. Kimura, S. N. Rai, H.-P. Liebermann, R. J. Buenker, H. Suno and P. C. Stancil, **Charge transfer and excitation in H<sup>+</sup> + CH<sub>3</sub> collisions below 10 keV, *Phys. Rev. A* **78**, 012708, 1-8 (2008).**
- 488 C. H. Liu, Y. Z. Qu, L. Liu, J. G. Wang, Y. Li, H.-P. Liebermann, P. Funke and R. J. Buenker, **Charge transfer and excitation in slow proton collisions with sodium, *Phys. Rev. A* **78**, 024703, 1-4 (2008).**
- 489 R. J. Buenker, **Gravitational and kinetic scaling of physical units, *Apeiron* **15**, 382-413 (2008).**
- 490 R. J. Buenker, **Extension of Schiff's gravitational scaling method to compute the precession of the perihelion of Mercury, *Apeiron* **15**, 509-532 (2008).**
- 491 M. V. Khoma, O. M. Karbovanets, M. I. Karbovanets and R. J. Buenker, **On the semiclassical approach in the theory of ion-diatom exchange interaction: application for charge exchange reactions, *Phys. Scripta* **78**, 065201, 1-10 (2008).**

- 492 R. J. Buenker, **Simultaneity and the constancy of the speed of light: Normalization of space-time vectors in the Lorentz transformation**, *Apeiron* **16**, 96-146 (2009).
- 493 C. Y. Lin, P. C. Stancil, H.-P. Liebermann, P. Funke and R. J. Buenker, **Inelastic processes in collisions of Na(3s,3p) with He at thermal energies**, *Phys. Rev. A* **78**, 052706, 1-7( 2008).
- 494 A. B. Alekseyev, H.-P. Liebermann and R. J. Buenker, **On the ultraviolet photofragmentation of  $\text{CH}_3\text{Xe}^+$** , *J. Chem. Phys.* **130**, 024309, 1-8 (2009).
- 495 M. V. Khoma, M. Imai, O. M. Karbovanets, Y. Kikuchi, M. Saito, Y. Haruyama,M. I. Karbovanets, I. Yu Kretinin, A. Itoh and R. J. Buenker, **Charge transfer processes in collisions of slow highly charged ions with polar molecules CO and  $\text{C}_3\text{H}_8$** , *J. Phys. Conf. Series* **163**, 012055, 1-4 (2009).
- 496 R. J. Buenker and H.-P. Liebermann, **Configuration interaction calculations of annihilation rates for positronic complexes of alkali hydrides**, *Nucl. Instr. and Meth. in Phys. Res. B* **267**, 763-767 (2009).
- 497 L. B. Zhao, D. C. Joseph, B. C. Saha, H.-P. Liebermann, P. Funke and R. J. Buenker, **Comparative study of quantal and semiclassical treatments of charge transfer between  $\text{O}^+$  and He**, *Phys. Rev. A* **79**, 034701, 1-4 (2009).
- 498 C. H. Liu, Y. Z. Qu, Y. Zhou, J. G. Wang, Y. Li and R. J. Buenker, **Radiative charge transfer in collisions of  $\text{H}^+$  with Na at very low energies**, *Phys. Rev. A* **79**, 042706, 1-5 (2009).
- 499 S. O. Adamson, R. J. Buenker, G. V. Golubkov, M. G. Golubkov and A. I. Dement'ev, **Laser stimulation of low-temperature dissociative recombination of electrons and oxygen molecular ions**, *Russ. J. Phys. Chem. B* **3**, No. 2, 195-210 (2009).
- 500 R.J. Buenker, **On the asymmetry in relativistic Doppler shifts caused by time dilation: proposed two-way experiment**, *Apeiron* **16**, 203-224 (2009).
- 501 Y. Wu, Y. Y. Qi, S. Y. Zou, J. G. Wang, Y. Li, R. J. Buenker and P. C. Stancil, **Quantum-mechanical calculations of charge transfer in collisions of  $\text{O}^{3+}$  with He**, *Phys. Rev. A.* **79**, 062711, 1-9 (2009).
- 502 Y. Wu, Y. Y. Qi, J. Yan, J. G. Wang, Y. Li, R. J. Buenker, D. Kato and P. S. Krstic, **Low-energy electron capture in collisions of  $\text{C}^{3+}$  with He**, *Phys. Rev. A.* **80**, 022715, 1-7 (2009).
- 503 M. Honigmann. R. J. Buenker and H.-P. Liebermann, **Complex MRD-CI calculations employing a coupled diabatic representation for the  ${}^2\Pi_g$  resonance states of  $\text{N}_2^-$** , *J. Chem. Phys.* **131**, 034303, 1-8 (2009).

- 504 C. H. Liu, Y. Z. Qu, J. G. Wang, Y. Li and R. J. Buenker, **Radiative charge transfer and radiative association of protons colliding with Na at low energies**, *Phys. Lett. A.* **373**, 3761-3763 (2009).
- 505 R. J. Buenker and H.-P. Liebermann, **Configuration interaction calculations of potential curves and annihilation rates for positronic complexes of alkali oxides**, *J. Chem. Phys.* **131**, 114107, 1-9 (2009).
- 506 C. H. Liu, Y. Z. Qu, J. G. Wang, Y. Li and R. J. Buenker, **Charge transfer and association of protons colliding with potassium from very low to intermediate energies**, *Phys. Rev. A.* **81**, 012707, 1-8 (2010).
- 507 A. Devdariani, A. K. Belyaev, A. B. Alekseyev, H.-P. Liebermann and R. J. Buenker, ***Ab initio* study of the lifetime of weakly bound He( $2^1S$ )-Ne molecules**, *Mol. Phys.* **108**, 757-762 (2010).
- 508 X. J. Liu, Y. Z. Qu, B. J. Xiao, C. H. Liu, Y. Zhou, J. G. Wang and R. J. Buenker, **Radiative charge transfer and radiative association in  $\text{He}^+ + \text{Ne}$  collisions**, *Phys. Rev. A* **81**, 022717, 1-8 (2010).
- 509 D. B. Kokh, H.-P. Liebermann and R. J. Buenker, **Photodissociation of  $\text{CH}_3\text{Cl}$ ,  $\text{C}_2\text{H}_5\text{Cl}$ , and  $\text{C}_6\text{H}_5\text{Cl}$  on the Ag(111) surface: Ab initio embedded cluster and configuration interaction study**, *J. Chem. Phys.* **132**, 074707, 1-10. (2010).
- 510 X. J. Liu, Y. Z. Qu, B. J. Xiao, C. H. Liu, Y. Zhou, J. G. Wang and R. J. Buenker, ***Ab initio* calculations of charge transfer in  $\text{He}^+$  colliding with Ne**, *J. Phys. B: At. Mol. Opt. Phys.* **43**, 085207, 1-7 (2010).
- 511 R. J. Buenker, **Time dilation and the concept of an objective rest system**, *Apeiron* **17**, 99-125 (2010).
- 512 M. Honigmann, H.-P. Liebermann and R. J. Buenker, **Use of complex configuration interaction calculations and the stationary principle for the description of metastable electronic states of  $\text{HCl}^-$** , *J. Chem. Phys.* **133**, 044305, 1-15 (2010).
- 513 G. V. Golubkov, M. G. Golubkov and R. J. Buenker, **Laser control of the low-temperature  $e^- + \text{O}_2^+$  reaction**, *J. Experimental and Theoretical Physics* **112**, 187-192 (2011).
- 514 M. Tachikawa, Y. Kita, and R. J. Buenker, **Bound states of positron with nitrile species with a configuration interaction multi-component molecular orbital approach**, *Phys. Chem. Chem. Phys.* **13**, 2701-2705 (2011).
- 515 A. B. Alekseyev, H.-P. Liebermann and R. J. Buenker, ***Ab initio* configuration interaction study of the B- and C-band photodissociation of methyl iodide**, *J. Chem. Phys.* **134**, 044303, 1-8 (2011).

- 516 V. Rai-Constapel, H.-P. Liebermann, A. B. Alekseyev and R. J. Buenker, **Configuration interaction study including the effects of spin-orbit coupling for the electronic states of the LiX molecules (X=C, Si, Ge, Sn)**, *Mol. Phys.* **109**, 975-985 (2011)
- 517 L. Pichl, M. Kimura, Y. Li and R.J. Buenker, **Branching ratios for secondary processes of water ions induced by proton beams in radiation therapy of cancer**, *IEEE Trans. Nucl. Sci.* **51**, 1407-1411 (2004).
- 518 R. J. Buenker, Y. Li, H.-P. Liebermann and M. Honigmann, **Use of Gauss-Hermite quadrature to approximate the asymptotic behaviour of vibronic resonance wave functions**, accepted for publication in *Khim. Fys.* (2011).
- 519 R. J. Buenker, H.-P. Liebermann and M. Kimura, **Configuration interaction calculations of cross sections for proton stopping reactions**, accepted for publication in *Int. J. Rad. Biol.* (2011).
- 520 Y. Wu, P. C. Stancil, H.-P. Liebermann, P. Funke, S.N. Rai, R. J. Buenker, D. R. Schultz, Y. Hui, I. N. Draganic and C. C. Havener, **Theoretical investigation of charge transfer between N<sup>6+</sup> and atomic hydrogen**, accepted for publication in *Phys. Rev. A* (2011).
- 521 A. Z. Devdariani, A. K. Belyaev, A. B. Alekseyev, H.-P. Liebermann and R. J. Buenker, **Ab initio study of the transition moments of weakly bound He(2<sup>1</sup>S)-Ne molecules: Temperature Dependence of Cross Sections**, accepted for publication in *Khim. Fys.* (2011).
- 522 G. V. Golubkov, M. G. Golubkov and R. J. Buenker, **Laser control of the low-temperature e<sup>-</sup> + O<sub>2</sub><sup>+</sup> reaction**, accepted for publication in *Khim. Fys.* (2011).
- 523 N. S. Malyshev, G. V. Golubkov, M. G. Golubkov and R. J. Buenker, **Potential energy surfaces of the K\*\*<sup>(n,l)</sup> + He system**, accepted for publication in *Khim. Fys.* (2011).
- 524 M. Honigmann, R. J. Buenker and H.-P. Liebermann, **Complex configuration interaction calculations of the cross sections for the dissociative attachment process e<sup>-</sup> + F<sub>2</sub> → F<sub>2</sub><sup>-</sup> → F + F<sup>-</sup>**, submitted for publication in *J. Comp. Chem.* (2011).