

List of Publications – Sean A. Peebles

(Undergraduate co-authors are underlined>

1. Rotational Spectrum of HCN–HI and a Comparison of Properties in the Series HCN–HX, P.W. Fowler, A.C. Legon and S.A. Peebles, *Chem. Phys. Lett.*, **226**, (1994), 501-508.
2. A Distributed Electrostatic Model for Field Gradients at Nuclei in van der Waals Molecules: Application to Complexes of HCl, A.D. Buckingham, P.W. Fowler, A.C. Legon, S.A. Peebles and E. Steiner, *Chem. Phys. Lett.*, **232**, (1995), 437-444.
3. Electric and Magnetic Properties of the BrCl Molecule, P.W. Fowler, A.C. Legon, S.A. Peebles and E. Steiner, *Chem. Phys. Lett.*, **238**, (1995), 163-167.
4. Anisotropic Repulsion in Complexes B–Cl₂ and B–HCl: the Shape of the Chlorine Atom-in-a-Molecule, S.A. Peebles, P.W. Fowler and A.C. Legon *Chem. Phys. Lett.*, **240**, (1995), 130-134.
5. Nuclear Quadrupole Coupling Constants in Complexes B–X₂: Sternheimer-Type Properties of Free X₂ from Experimental Intramolecular Charge Shifts, P.W. Fowler, A.C. Legon and S.A. Peebles, *Mol. Phys.*, **88**, (1996), 987-996.
6. Electric Field Gradients and Sternheimer-Type Properties of the BrCl Molecule: Correlated, Relativistic, Ab Initio Calculations and Modelling of Nuclear Quadrupole Coupling Constants in Complexes B–BrCl, P.W. Fowler, S.A. Peebles, A.C. Legon and A.J. Sadlej, *Chem. Phys. Lett.*, **257**, (1996), 249-256.
7. Cation Polarization and the Crystal Structure of SnO, M. Wilson, P.A. Madden, S.A. Peebles and P.W. Fowler, *Mol. Phys.*, **88**, (1996), 1143-1153.
8. A Sternheimer-like Response Property of the Bromine Molecule: Electric Field Dependence of the Br Field Gradient, P.W. Fowler, S.A. Peebles and A.C. Legon, *Adv. Quant. Chem.*, **28**, (1997), 247-256.
9. The Structure of the Cyclopropane–Methanol Complex, S.E. Forest, S.A. Peebles, L.H. Sun, A.M. Andrews and R.L. Kuczkowski, *J. Mol. Struct.*, **413-414**, (1997), 255-263.
10. An Electrostatic Interaction Model Applied to Complexes of Sulfur Dioxide, S.A. Peebles and R.L. Kuczkowski, *J. Mol. Struct.*, **436-437**, (1997), 59-67.
11. Rotational Spectrum and Structure of the OCS–(CO₂)₂ Trimer, S.A. Peebles and R.L. Kuczkowski, *Chem. Phys. Lett.*, **286**, (1998), 421-424.

12. The Structure and Dipole Moment of the Argon–Fluorobenzene Dimer, R.A. Appleman, S.A. Peebles and R.L. Kuczkowski, *J. Mol. Struct.*, **446**, (1998), 55-61.
13. Application of Interaction Models to Complexes of Sulfur Dioxide, S.A. Peebles and R.L. Kuczkowski, *J. Mol. Struct.*, **447**, (1998), 151-158.
14. Rotational Spectrum and Structure of the OCS–(CO₂)₂ Trimer, S.A. Peebles and R.L. Kuczkowski, *J. Chem. Phys.*, **109**, (1998), 5276-5282.
15. Rotational Spectrum and Structure of the (OCS)₂–CO₂ Trimer, S.A. Peebles and R.L. Kuczkowski, *J. Phys. Chem. A*, **102**, (1998), 8091-8096.
16. The Structure of the Boron Trifluoride–Sulfur Dioxide Complex, S.A. Peebles, L.H. Sun, R.L. Kuczkowski, L.M. Nxumalo and T.A. Ford, *J. Mol. Struct.*, **471**, (1998), 235-242.
17. Aromatic–Rare Gas Complexes: The Microwave Spectrum and Structure of the Fluorobenzene–Neon Dimer, R.J. Wilson, S.A. Peebles, S. Antolínez, M. Eugenia Sanz and R.L. Kuczkowski, *J. Phys. Chem. A*, **102**, (1998), 10630-10635.
18. Rotational Spectrum, Structure and Modeling of the SO₂–CS₂ Complex, S.A. Peebles, L.H. Sun and R.L. Kuczkowski, *J. Chem. Phys.*, **110**, (1999), 6804-6811.
19. The Microwave Spectrum and Structure of the Acetylene–OCS Dimer, S.A. Peebles and R.L. Kuczkowski, *J. Phys. Chem. A*, **103**, (1999), 3884-3889.
20. Microwave Spectrum and Structure of the (CO₂)₂–N₂O Complex, R.A. Peebles, S.A. Peebles and R.L. Kuczkowski, *Mol. Phys.*, **96**, (1999), 1355-1365.
21. The Rotational Spectrum of the Acetylene–Carbonyl Sulfide Trimer: HCCH–(OCS)₂, S.A. Peebles and R.L. Kuczkowski, *Chem. Phys. Lett.*, **308**, (1999), 21-25.
22. Rotational Spectrum, Structure and Modeling of the SO₂–OCS Complex, S.A. Peebles, L.H. Sun, I.I. Ioannou and R.L. Kuczkowski, *J. Mol. Struct.*, **486**, (1999), 211-223.
23. Rotational Spectrum, Structure and Modeling of an Isomer of the HCCH–OCS Dimer, S.A. Peebles and R.L. Kuczkowski, *Chem. Phys. Lett.*, **312**, (1999), 357-361.
24. Rotational Spectrum, Structure and Modeling of the HCCH–(OCS)₂ Trimer: Observation of a Polar OCS Dimer Fragment, S.A. Peebles and R.L. Kuczkowski, *J. Chem. Phys.*, **111**, (1999), 10511-10519.
25. Isotopic Studies, Structure and Modeling of the Nitrous Oxide–Acetylene Complex, R.A. Peebles, S.A. Peebles, R.L. Kuczkowski and H.O. Leung, *J. Phys. Chem. A*, **103**, (1999), 10813-10818.

26. Equilibrium Structure of *cis*-hex-3-ene-1,5-diyne and Relevance to the Bergman Cyclization, R.J. McMahon, R.J. Halter, R.L. Fimmen, R.J. Wilson, S.A. Peebles, R.L. Kuczkowski and J.F. Stanton, *J. Am. Chem. Soc.*, **122**, (2000), 939-949.
27. Rotational Spectrum and Modeling of the OCS–(HCCH)₂ Trimer, S.A. Peebles and R.L. Kuczkowski, *J. Mol. Struct. (Theochem)*, **500**, (2000), 391-402.
28. The Rotational Spectrum and Structure of 1,2-Dichloro-3,3,4,4-tetrafluorocyclobutene: Comparison of Spectroscopy, Diffraction and *Ab Initio* Results, A.W. van Wynsberghe, S.A. Peebles, R.A. Peebles and R.L. Kuczkowski, *J. Phys. Chem.*, **104**, (2000), 8702-8708
29. The Microwave Spectrum and Structure of the Chlorobenzene–Argon Dimer, J.J. Oh, I. Park, R.J. Wilson, S.A. Peebles and R.L. Kuczkowski, *J. Chem. Phys.*, **113**, (2000), 9051-9059
30. Rotational Spectrum, Structure and Internal Motions of the Ethylene–OCS Weakly Bound Dimer, S.A. Peebles and R.L. Kuczkowski, *Mol. Phys.*, **99**, (2001), 225-237
31. The Rotational Spectrum and Structure of the Chlorobenzene–Neon van der Waals Dimer, J.J. Oh, I. Park, S.A. Peebles and R.L. Kuczkowski, *J. Mol. Struct.*, **599**, (2001), 15-22.
32. Microwave Spectra and Molecular Structures of (*Z*)-Pent-2-en-4-ynenitrile and Maleonitrile, R.J. Halter, R.L. Fimmen, R.J. McMahon, S.A. Peebles, R.L. Kuczkowski and J.F. Stanton, *J. Am. Chem. Soc.*, **123**, (2001), 12353-12363.
33. Rotational Spectrum and Dipole Moment of 1-chloro-4-fluorobenzene, S.A. Peebles and R.A. Peebles, *J. Mol. Struct.*, **607**, (2002), 19-29.
34. Rotational Spectrum and Structure of the (OCS)₂–C₂H₄ Trimer: Example of a Polar OCS Dimer, R.A. Peebles, S.A. Peebles and R.L. Kuczkowski, *J. Mol. Struct.*, **612**, (2002), 261–276.
35. Structures of Diethynyl Sulfide and Bis(phenylethynyl) Sulfide, A.J., Matzger, K.D. Lewis, C.E. Nathan, S.A. Peebles, R.A. Peebles, R.L. Kuczkowski, J.F. Stanton, J.J. Oh, *J. Phys. Chem. A*, **106**, (2002), 12110–12116.
36. The Microwave Spectrum, *Ab Initio* Analysis and Structure of the Fluorobenzene-Hydrogen Chloride Complex, M. Eugenia Sanz, S. Antolínez, J.L. Alonso, J.C. Lopez, R.L. Kuczkowski, S.A. Peebles, R.A. Peebles, F.C. Boman, E. Kraka and D. Cremer, *J. Chem. Phys.*, **118**, (2003), 9278–9290.
37. Determination of the Heavy Atom Structure of Bromobenzene by Rotational Spectroscopy, S.A. Peebles and R.A. Peebles, *J. Mol. Struct.*, **657**, (2003), 107–116.

38. Determination of the Heavy Atom Structure of 3-butyn-1-ol by Microwave Spectroscopy, E.D. Slagle, R.A. Peebles and S.A. Peebles, *J. Mol. Struct.*, **693**, (2004), 167-174.
39. The Dimethyl Ether–OCS dimer: Rotational Spectrum, Structure and ab initio calculations, J.J. Newby, R.A. Peebles and S.A. Peebles, *J. Phys. Chem. A*, **108**, (2004), 7372-7378.
40. Structure of the Dimethyl Ether–CO₂ van der Waals Complex from Microwave Spectroscopy, J.J. Newby, R.A. Peebles and S.A. Peebles, *J. Phys. Chem. A*, **108**, (2004), 11234-11240.
41. Rotational Spectrum, Structure and Modeling of the OCS–CS₂ van der Waals Complex, J.J. Newby, M.M. Serafin, R.A. Peebles and S.A. Peebles, *Phys. Chem. Chem. Phys.*, **7**, (2005), 487-492.
42. Heavy atom structure and conformer stabilities of cyclopropyl carbinol from rotational spectroscopy and ab initio calculations, J.J. Newby, R.A. Peebles and S.A. Peebles, *J. Mol. Struct.*, **740**, (2005), 133-142.
43. Rotational Spectrum of the Dimethyl Ether–Acetylene Complex: Evidence for an Effective C_{2v} Geometry, J.J. Newby, M.M. Serafin, R.A. Peebles and S.A. Peebles, *J. Phys. Chem. A*, **109**, (2005), 5316-5322.
44. Tunneling Motions and the Barrier to Inversion in the Dimethyl Ether–CS₂ van der Waals Dimer, S.A. Peebles, R.A. Peebles, J.J. Newby and M.M. Serafin, *Chem. Phys. Lett.*, **410**, (2005), 77-81.
45. Rotational Spectrum and Inversion Motions in the Neon–Dimethyl Sulfide Complex, S.A. Peebles, R.A. Peebles, Y. Tatamitani and Y. Kawashima, *J. Phys. Chem. A*, **110**, (2006), 7080-7085.
46. Rotational Spectrum and Structure of the Carbonyl Sulfide-Trifluoromethane Weakly Bound Dimer, M.M. Serafin and S.A. Peebles, *J. Phys. Chem. A*, **110**, (2006), 11938-11943.
47. Isotopic Studies and Refined Structure for the Dimethyl Ether–CS₂ Dimer, S.A. Peebles and R.A. Peebles, *J. Mol. Struct.*, **830**, (2007), 176-181.
48. Oxygen-17 Hyperfine Structures in the Pure Rotational Spectra of SrO, SnO, BaO, HfO And ThO, C.T. Dewberry, K.C. Etchison, G.S. Grubbs II, R.A. Powoski, M.M. Serafin, S.A. Peebles and S.A. Cooke, *Phys. Chem. Chem. Phys.*, **9**, (2007), 5897-5901.
49. Concerning the Electron Density at the Pb Nucleus in PbO as a Function of Bond Length, M.M. Serafin, S.A. Peebles, C.T. Dewberry, K.C. Etchison, G.S. Grubbs II, R.A. Powoski, S.A. Cooke, *Chem. Phys. Lett.*, **449**, (2007), 33-37.

50. The ^{115}Sn , ^{117}Sn and ^{119}Sn nuclear spin-rotation constants in stannous monoxide, SnO , and a new multi-isotopomer analysis. C.T. Dewberry, K.C. Etchison, G.S. Grubbs II, R.A. Powoski, M.M. Serafin, S.A. Peebles, and S.A. Cooke, *J. Mol. Spectrosc.*, **248**, (2008), 20-25.
51. Microwave Spectrum, Dipole Moment and Internal Dynamics of the Methyl Fluoride–Carbonyl Sulfide Weakly Bound Complex, M.M. Serafin, S.A. Peebles, *J. Phys. Chem. A*, **112**, (2008), 1473-1479.
52. Internal Rotation Effects in the Pulsed Jet Rotational Spectrum of the Trifluoromethane–Carbon Dioxide Dimer, M.M. Serafin, R.A. Peebles and S.A. Peebles, *J. Mol. Spectrosc.*, **250**, (2008), 1-7.
53. The Pure Rotational Spectrum of Pivaloyl Chloride, $(\text{CH}_3)_3\text{CCOCl}$, between 800 MHz and 18800 MHz, G.S. Grubbs II, C.T. Dewberry, K.C. Etchison, M.M. Serafin, S.A. Peebles, S.A. Cooke, *J. Mol. Spectrosc.*, (2008), in press.