

## List of Publications of Thom H. Dunning, Jr.

## Peer-Reviewed Journals

1. "Non-Empirical Calculations on Excited States: The Ethylene Molecule," T. H. Dunning, Jr. and V. McKoy, *J. Chem. Phys.*, **47**, 1735–1747 (1967).
2. "Localized Orbitals. I. Sigma Bonds," J. H. Letcher and T. H. Dunning, Jr., *J. Chem. Phys.*, **48**, 4538–4543 (1968).
3. "Non-Empirical Calculations on Excited States: The Formaldehyde Molecule," T. H. Dunning, Jr. and V. McKoy, *J. Chem. Phys.*, **48**, 5263–5270 (1968).
4. "The Formaldehyde Molecule in a Gaussian Basis. A Self-Consistent Field Calculation," N. W. Winter, T. H. Dunning, Jr., and J. H. Letcher, *J. Chem. Phys.*, **49**, 1871–1877 (1968).
5. "The Formaldehyde Molecule in a Gaussian Basis. One-Electron Properties," T. H. Dunning, Jr., N. W. Winter, and V. McKoy, *J. Chem. Phys.*, **49**, 4128–4140 (1968).
6. "Characterization of Ground State Wavefunctions by Measured Electronic Properties. II. Dipole Moment and Field Gradient of Nitrogen Trifluoride," M. L. Unland, T. H. Dunning, Jr., and J. R. van Wazer, *J. Chem. Phys.*, **50**, 3208–3214 (1969).
7. "The Orthogonality Constrained Basis Set Expansion Method for Treating Off-Diagonal Lagrange Multipliers in the Calculation of Electronic Wavefunctions," W. J. Hunt, T. H. Dunning, Jr., and W. A. Goddard, III, *Chem. Phys. Lett.*, **3**, 606–610 (1969).
8. "The Theoretical Description of the ( $\pi\pi^*$ ) Excited States of Ethylene," T. H. Dunning, Jr., W. J. Hunt, and W. A. Goddard, III, *Chem. Phys. Lett.*, **4**, 147–150 (1969).
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10. "The Incorporation of Quadratic Convergence into Open-Shell Self-Consistent Field Equations," W. J. Hunt, W. A. Goddard, III, and T. H. Dunning, Jr., *Chem. Phys. Lett.*, **6**, 147–151 (1970).
11. "Gaussian Basis Sets for Use in Molecular Calculations. I. Contraction of (9s5p) Atomic Basis Sets for the First Row Atoms," T. H. Dunning, Jr., *J. Chem. Phys.*, **53**, 2823–2833 (1970).
12. "Comparison of Slater and Contracted Gaussian Basis Sets in SCF and CI Calculations on H<sub>2</sub>O," R. P. Hosteny, R. R. Gilman, T. H. Dunning, Jr., A. Pipano, and I. Shavitt, *Chem. Phys. Lett.*, **7**, 325–328 (1970).
13. "Gaussian Basis Functions for Use in Molecular Calculations. Contraction of (12s9p) Atomic Basis Sets for the Second-Row Atoms," T. H. Dunning, Jr., *Chem. Phys. Lett.*, **7**, 423–427 (1970).
14. "Accelerating the Convergence of Matrix Hartree–Fock Calculations," N. W. Winter and T. H. Dunning, Jr., *Chem. Phys. Lett.*, **8**, 169–172 (1971).
15. "Gaussian Basis Functions for Use in Molecular Calculations. III. Contraction of (10s6p) Atomic Basis Sets for the First-Row Atoms," T. H. Dunning, Jr., *J. Chem. Phys.*, **55**, 716–723 (1971).
16. "Formaldehyde Molecule in a Gaussian Basis: Electronic Density," T. H. Dunning, Jr. and N. W. Winter, *J. Chem. Phys.*, **55**, 3360–3371 (1971).
17. "Hartree–Fock Calculation of the Barrier to Internal Rotation in Hydrogen Peroxide," T. H. Dunning, Jr. and N. W. Winter, *Chem. Phys. Lett.*, **11**, 194–195 (1971).
18. "Gaussian Basis Functions for Use in Molecular Calculations. IV. Representation of Polarization Functions for the First-Row Atoms and Hydrogen," T. H. Dunning, Jr., *J. Chem. Phys.*, **55**, 3958–3966 (1971).
19. "Multiconfiguration Wavefunctions for the Lowest ( $\pi\pi^*$ ) Excited States of Ethylene," C. F. Bender, T. H. Dunning, Jr., H. F. Schaefer III, W. A. Goddard III, and W. J. Hunt, *Chem. Phys. Lett.*, **15**, 171–178 (1972).
20. "Ab Initio and Semi-Empirical Calculations on the Static Potential for Electron Scattering Off the Nitrogen Molecule," D. G. Truhlar, F. A. Van Catledge, and T. H. Dunning, Jr., *J. Chem. Phys.*, **57**, 4788–4799 (1972).
21. "Near Hartree–Fock Calculations on the Ground State of the Water Molecule: Energies, Ionization Potentials, Force Constants, and One-Electron Properties," T. H. Dunning, Jr., R. M. Pitzer, and S. Aung, *J. Chem. Phys.*, **57**, 5044–5051 (1972).
22. "Assignment of the Low-Lying  $\pi$ -Electron States of *trans*-Butadiene," T. H. Dunning, Jr., R. P. Hosteny, and I. Shavitt, *J. Am. Chem. Soc.*, **95**, 5067–5068 (1973).
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24. "Theoretical Evidence for Bound Electronic States of Ozone," P. J. Hay, T. H. Dunning, Jr., and W. A. Goddard, III, *Chem. Phys. Lett.*, **23**, 457–462 (1973).
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26. "New Electronic States of N<sub>2</sub><sup>+</sup>," D. C. Cartwright and T. H. Dunning, Jr., *J. Phys.*, **B8**, L100–L104 (1975).
27. "Configuration Interaction Studies of O<sub>3</sub> and O<sub>3</sub><sup>+</sup>," P. J. Hay, T. H. Dunning, Jr., and W. A. Goddard, III, *J. Chem. Phys.*, **62**, 3912–3924 (1975).
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29. "Theoretical Determination of the Barriers to Internal Rotation in Hydrogen Peroxide," T. H. Dunning, Jr. and N. W. Winter, *J. Chem. Phys.*, **63**, 1847–1855 (1975).
30. "The Electronic States of KrF," T. H. Dunning, Jr. and P. J. Hay, *Appl. Phys. Lett.*, **28**, 649–651 (1976).
31. "Generalized Valence Bond Calculations on the Ground State (X<sup>1</sup> $\Sigma_g^+$ ) of Nitrogen," T. H. Dunning, Jr., D. C. Cartwright, W. J. Hunt, P. J. Hay, and F. W. Bobrowicz, *J. Chem. Phys.*, **64**, 4755–4766 (1976).
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33. "The Electronic Structure of Pyrazine. Configuration Interaction Calculations Using an Extended Basis," W. R. Wadt, W. A. Goddard, III, and T. H. Dunning, Jr., *J. Chem. Phys.*, **65**, 438–445 (1976).

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38. "Gaussian Basis Sets for the Atoms Gallium Through Krypton," T. H. Dunning, Jr., *J. Chem. Phys.*, **66**, 1382–1383 (1977).
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