

1. Papers in Refereed Journals

1. "Nonorthonormal CI for molecular excited states. I. The sudden polarization effect in 90° twisted ethylene",
I.D. Petsalakis, G. Theodorakopoulos, C.A. Nicolaidis, R.J. Buenker and S.D. Peyerimhoff,
J. Chem. Phys. 81, 3161 (1984).
2. "Non-orthonormal CI for molecular excited states. II. The zwitterionic states of terminally twisted butadiene",
I.D. Petsalakis, G. Theodorakopoulos, C.A. Nicolaidis and R.J. Buenker,
J. Chem. Phys. 81, 5952 (1984).
3. "MRD-CI calculations on the potential energy curves of the ground and excited electronic states of the noble-gas hydrides, HeH, NeH and ArH",
G. Theodorakopoulos, S.C. Farantos, R.J. Buenker and S.D. Peyerimhoff,
J. Phys. B 17, 1453 (1984).
4. "Bending potentials for H₂O in the ground and the first six singlet excited states",
G. Theodorakopoulos, I.D. Petsalakis, R.J. Buenker and S.D. Peyerimhoff,
Chem. Phys. Lett. 105, 253 (1984).
5. "Theoretical and experimental ionization potentials of (CH₃)₂S and (CH₃)₂SO. The effect of substituents R on the sulphur ESCA shifts in the series R₂S, R₂SO, R₂SO₂",
G. Theodorakopoulos, I.D. Petsalakis, I.G. Csizmadia and M.A. Robb,
Theochem-J. Mol. Struct. 110, 381 (1984).
6. "Theory of chemical reactions of vibronically excited H₂ ($B^1\Sigma_u^+$). I. Prediction of a strongly bound excited state of H₄",
C.A. Nicolaidis, G. Theodorakopoulos and I.D. Petsalakis,
J. Chem. Phys. 80, 1705 (1984).
7. "Theory of chemical reactions of vibronically excited H₂($B^1\Sigma_u^+$). II. Noble gas dihydrides",
C.A. Nicolaidis and A. Zdetsis,
J. Chem. Phys. 80, 1900 (1984).
8. "Theory of chemical reactions of vibronically excited H₂ ($B^1\Sigma_u^+$). III. Formation of bound excited states of the (H₂)₂, (H₂)₃, and (H₂)₅ clusters",
C.A. Nicolaidis, I.D. Petsalakis and G. Theodorakopoulos,
J. Chem. Phys. 81, 748 (1984).
9. "The variation in the second hyperpolarisability of cyclobutane and cyclopentane through inversion, and an analysis of the contributions to this property",

J. Waite and M.G. Papadopoulos,
Can. J. Chem. 62, 1736 (1984).

10. "The 2nd hyperpolarizability of 1-nitronaphthalene",
J. Waite and M.G. Papadopoulos,
J. Chem. Phys. 80, 3503 (1984).

11. "A study of molecular polarisation The effect of lithiation on the hyperpolarisabilities of $\text{CH}_n\text{Li}_{6-n}$ ",
J. Waite and M.G. Papadopoulos,
J. Mol. Structure 125, 155 (1984).

12. "Electric second hyperpolarizability as a novel probe to the stability of dianions. Case study: four conformers of $\text{C}_6\text{H}_8^{2-}$ ",
J. Waite and M.G. Papadopoulos,
J. Org. Chem. 49, 3837 (1984).

13. "The variation of calculated electric polarizabilities and hyperpolarizabilities, in cycloocta-1,5-diene, annulene, their anions and several of their derivatives, induced by changes in molecular-structure and charge - a comparative-study",
J. Waite and M.G. Papadopoulos,
Theochem-J. Mol. Struct. 17, 247 (1984).

14. "Analytical ab initio potential-energy surfaces for the ground and the first singlet excited states of HeH_2 ",
S.C. Farantos, J.N. Murrell and S. Carter,
Chem. Phys. Lett. 108, 367 (1984).

15. "Vibrational chaos in KCN: A comparison of quantum and classical calculations",
J. Tennyson and S.C. Farantos,
Chem. Phys. Lett. 109, 160 (1984).

16. "Rotationally inelastic collisions of LiH with He: Quasiclassical dynamics of atom-rigid rotor trajectories",
A. Metropoulos and D.M. Silver,
J. Chem. Phys. 81, 1682 (1984).

17. "Rotational energy transfer in the helium-nitrogen collision system",
A. Metropoulos,
J. Phys. Chem. 88, 1 (1984).

18. "Electron correlation and relativistic effects on the energies and widths of doubly excited-states of He",
G. Aspromallis, Y. Komninos and C. A. Nicolaides,
J. Phys. B 17, L151 (1984).

19. "Autoionization widths of the doubly excited-states of Be^+ ",
G. Aspromallis and C.A. Nicolaides,
J. Phys. B 17, L249 (1984).
20. "Localized and asymptotic electron correlation in autoionising states in terms of complex coordinates",
T. Mercouris and C.A. Nicolaides,
J. Phys. B 17, 4127 (1984).
21. "Fine and hyperfine structure of the two lowest bound-states of Be^- and their first two ionization thresholds",
D.R. Beck and C.A. Nicolaides,
Int. J. Quantum Chem. 26, 467 (1984).
22. "Many-electron theory of auto-ionizing states using complex coordinates - the position and the partial and total widths of the Ne^+ 1s hole state",
C.A. Nicolaides, T. Mercouris and Y. Komninos,
Int. J. Quantum Chem. 26, 1017 (1984).
23. "Generalized oscillator-strengths and photoionization of alkali-metal atoms",
S.N. Tiwary and C.A. Nicolaides,
Physica B & C 125, 379 (1984).
24. "Angular-dependence of the X-Ray Raman-scattering intensity from polycrystals",
A.N. Andriotis and C.A. Londos,
Solid State Commun. 49, 213 (1984).
25. "State-specific, many-electron theory of core levels in metals - the 1s binding-energy of Be metal",
C.A. Nicolaides, A.D. Zdetsis and A.N. Andriotis,
Solid State Commun. 50, 857 (1984).
26. "Interaction of Argon with the Al(100) surface",
A.N. Andriotis and C.A. Nicolaides,
Solid State Commun. 51, 251 (1984).
27. "Incorporation of lattice effects in surface-energy calculations",
A.N. Andriotis,
Surf. Sci. 138, 269 (1984).
28. "Quantum-mechanical treatment of cerous magnesium-nitrate in an external magnetic-field",
A.K. Theophilou and S. Thanos,
Phys. Rev. B 30, 6596 (1984).
29. "Electronic and vibrational-spectra of mixed-valence complexes with a metal-halide

chain",

G.C. Papavassiliou and C.S. Jacobsen,
J. Mol. Struct. 115, 37 (1984).

30. "Spectroscopic investigation of metal dimercaptodithiolenes and selenium analogs",
G.C. Papavassiliou, A.M. Cotsilios and C.S. Jacobsen,
J. Mol. Struct. 115, 41 (1984).

31. "Laser-Raman spectroscopic studies of the eggshell (Chorion) of Bombyx-Mori",
S.J. Hamodrakas, E.I. Kamitsos and A. Papanikolaou,
Int. J. Biol. Macromol. 6, 333 (1984).

32. "A Raman-study of lithium-fluoride containing fast ionic conducting glasses",
D.E. Turcotte, W.M. Risen and E.I. Kamitsos,
Solid State Commun. 51, 313 (1984).

2. Dissertations

a. PhD theses

1. "Quantum mechanical calculations of the electric polarizabilities and hyperpolarizabilities of a few organic molecules and anions",
J. Waite, University College of London (1984).

b. Honors theses

1. "Excimer lasers",
E. Asproulakis, Th. Zafiriou, supervisors A.C. Cefalas and G. Kourouklis, National Technical University of Athens (1984).