

1. "Theoretical prediction of new Kubas four centre H₂ complexes involving dimolybdate clusters", E. D. Simandiras and D. G. Liakos, *Chem. Phys. Lett.* **583**, 18 (2013)
2. "Which component of the quadruple bond breaks first upon protonation of octachlorodimetalate anions [MM'Cl₈]⁴⁻, M,M'=Mo, W?: a theoretical study of reactivity, mechanism and bonding", E. D. Simandiras, N. Psaroudakis and K. Mertis, *Polyhedron* **54**, 173 (2013)
3. "Modification of Wilkinson's catalyst with triphenyl phosphite: Synthesis, structure, ³¹P NMR and DFT study of trans-[RhCl(P(OPh)₃)(PPh₃)₂]", I. Choinopoulos, I. Papageorgiou, S. Coco, E. Simandiras and S. Koinis, *Polyhedron* **45**, 255 (2012)
4. "Theoretical Elucidation of a Classic Reaction: Protonation of the Quadruple Bond of the Octachlorodimolybdate(II,II) [Mo₂Cl₈]⁴⁻ Anion", E. D. Simandiras, M. Tsakiroglou, N. Psaroudakis, D. G. Liakos, and K. Mertis, *Inorg. Chem.*, **51**, 258 (2012)
5. "Structural properties of lithium metaphosphate glasses by ab initio molecular electronic structure calculations", D.G. Liakos and E.D. Simandiras *J. Non-Cryst. Solids* **354**, 1569 (2008).
6. "Theoretical Study of Glass Systems using Molecular Electronic Structure Theory. 2. Structure and Spectroscopy of the B₂O₃ Glass", D. G. Liakos and E. D. Simandiras, *J. Phys. Chem.* **A112**, 7881 (2008)
7. "Theoretical investigation of the stepwise hydrolysis of the [Re₃(μ-Cl₃)Cl₉]³⁻ Anion", D.G. Liakos, E.D. Simandiras, N. Psaroudakis and K. Mertis, *Inorg. Chem.*, **46**, 2167 (2007).
8. "A Theoretical Study of Glass Systems using ab initio molecular electronic structure theory I. Lithium Metaphosphate Glass", E. D. Simandiras and D. G. Liakos, *J. Phys. Chem. A* **108**, 3854 (2004).
9. "A theoretical study on the solvolytic reactivity of the [Re₃(μ-Cl₃)Cl₉]_n- clusters (n=3,4) using ab initio and density functional theory calculations", N. Psaroudakis, K. Mertis, D. G. Liakos and E. D. Simandiras, *Chem. Phys. Lett.* **369**, 490 (2003).
10. "Prediction of Nonclassical Hydrogen Complexes of Nontransition Metals", C. A. Nicolaides and E. D. Simandiras, *Comments Inorg. Chem.* **18**, 65 (1996).
11. "Prediction and Characterisation of Magnesium Fluoride Dimers and their Non-classical Hydrogen Complexes", E. D. Simandiras and C. A. Nicolaides, *Chem. Phys. Lett.* **223**, 233 (1994).
12. "Prediction of Non-transition-metal Hydrogen Complexes", C. A. Nicolaides and E. D. Simandiras, *Chem. Phys. Lett.* **196**, 213 (1992)
13. "Nonclassical Hydrogen Complexes of the Alkaline Earths", E. D. Simandiras and C. A. Nicolaides, *Chem. Phys. Lett.* **185**, 529 (1991)
14. "Structure and vibrational analysis of protonated hydrogen peroxide", P. Valtazanos, E. D. Simandiras and C. A. Nicolaides, *Chem. Phys. Lett.* **156**, 240 (1989).
15. "On the necessity of f basis functions for bending frequencies", E. D. Simandiras, J. E. Rice, T. J. Lee, R. D. Amos, and N. C. Handy, *J. Chem. Phys.* **88**, 3187 (1988).
16. "The structure and harmonic vibrational frequencies of the weakly bound complexes formed by HF with CO, CO₂, and N₂O", I. L. Alberts, N. C. Handy and E. D. Simandiras, *Theor. Chim. Acta* **74**, 415 (1988).

17. "Correlated ab initio harmonic frequencies and infrared intensities for furan, pyrrole and thiophene", E D Simandiras, R D Amos and N C Handy, *J. Phys. Chem.* **92**, 1739 (1988).
18. "Second-order perturbation theory and configuration interaction theory applied to medium-sized molecules: Cyclopropane, Ethyleneimine, Ethylene Oxide, Fluoroethane and Acetaldehyde", E D Simandiras, R D Amos, N C Handy, T J Lee, J E Rice, H F Schaefer, *J. Amer. Chem. Soc.* **110**, 1388 (1988).
19. "The structure and vibrational frequencies of the ArH_3^+ ion and its isotopomers", E D Simandiras, J F Gaw and N C Handy, *Chem. Phys. Lett.* **141**, 166 (1987).
20. "Accurate ab initio prediction of molecular geometries and spectroscopic constants using SCF and MP2 energy derivatives", N C Handy, J F Gaw and E D Simandiras, *J. Chem. Soc. Faraday Trans. II* **83**, 1577 (1987).
21. "Hydrogen-bonded complexes involving HF and HCl; the effects of electron correlation and anharmonicity", R D Amos, J F Gaw, N C Handy, E D Simandiras and K Somasundram, *Theor. Chim. Acta* **71**, 41 (1987).
22. "The analytic evaluation of second-order Moller-Plesset dipole moment derivatives", E D Simandiras, R D Amos and N C Handy, *Chem. Phys.* **114**, 9 (1987).
23. "On the high accuracy of MP2-optimised geometries and harmonic frequencies with large basis sets", E D Simandiras, R D Amos and N C Handy, *Chem. Phys. Lett.* **133**, 324 (1987).
24. "A theoretical study of the reaction of Ca ($4s4p\ ^3P$) with H_2 ", E D Simandiras and N C Handy, *J. Chem. Soc. Faraday Trans. II*, **82**, 269 (1986).
25. "The elimination of singularities in derivative calculations", N C Handy, R D Amos, J F Gaw, J E Rice and E D Simandiras, *Chem. Phys. Lett.* **120**, 151 (1985).

Conference Proceedings

26. "Techniques used in evaluating orbital and wavefunction coefficients and property derivatives", N C Handy, R D Amos, J F Gaw, J E Rice, E D Simandiras, T J Lee, R J Harrison, W D Laidig, G B Fitzgerald and R J Bartlett, in: P Jorgensen and J Simons (eds), *Geometrical Derivatives of Energy Surfaces and Molecular Properties* (NATO ASI, Reidel, Dordrecht, 1986).

In Press

27. "Synthesis, Characterization, and Theoretical Studies of Novel Phthalocyanine Complexes", A. Thimiopoulos, A. Vogiatzi, E. D. Simandiras, G. A. Mousdis and N. Psaroudakis, *Inorg. Chim. Acta*, accepted (2013).