

## Dr. Ioannis Kerkines

### *Publication list*

(Last updated: November 22, 2013)

#### **A. B.Sc. Thesis**

1. “Badger’s Rule”, Department of Chemistry, National and Kapodistrian University of Athens, Greece (Advisor: A. Mavridis) (1997).

#### **B. M.Sc. Thesis**

2. “Ab initio calculations on the LiHe, LiHe<sub>2</sub> and ScC<sup>+</sup> molecular systems”, Department of Chemistry, National and Kapodistrian University of Athens, Greece (Advisor: A. Mavridis) (1999).

#### **C. Ph.D. Thesis**

3. “I. A theoretical study of the TiC<sup>+</sup>, VC<sup>+</sup> and CrC<sup>+</sup> metal carbides. II. The bonding nature of the N<sub>5</sub><sup>+</sup> cation and related systems.”, Department of Chemistry, National and Kapodistrian University of Athens, Greece (Advisor: A. Mavridis) (2003).

#### **D. Publications in international refereed journals**

4. “Ab Initio Investigation of the LiHe X<sup>2</sup>Σ<sup>+</sup>, A<sup>2</sup>Π and B<sup>2</sup>Σ<sup>+</sup> States. A Basis Set Study.”, I. S. K. Kerkines and A. Mavridis, *J. Phys. Chem. A* **2000**, *104*, 408–412.

5. “Electronic Structure of Scandium and Titanium Carbide Cations, ScC<sup>+</sup> and TiC<sup>+</sup>. Ground and Low-Lying States.”, I. S. K. Kerkines and A. Mavridis, *J. Phys. Chem. A* **2000**, *104*, 11777–11785.

6. “An Accurate Description of the LiNe X  $^2\Sigma^+$ , A  $^2\Pi$  and B  $^2\Sigma^+$  States.”, I. S. K. Kerkines and A. Mavridis, *J. Phys. Chem. A* **2001**, *105*, 1983–1987.
7. “On the Bonding Nature of the  $N_5^+$  (=  $N(N_2)_2^+$ ) Cation and Related Species,  $N(CO)_x^+$ ,  $N(NH_3)_x^+$ , and  $NR_x^+$ ,  $x = 1, 2$ ; R = He, Ne, Ar, Kr. Do We Really Need the Resonance Concept?”, I. S. K. Kerkines, A. Papakondylis, and A. Mavridis, *J. Phys. Chem. A* **2002**, *106*, 4435–4442.
8. “Theoretical Investigation of the X  $^2\Sigma^+$ , A  $^2\Pi$  and B  $^2\Sigma^+$  States of LiAr and LiKr.”, I. S. K. Kerkines and A. Mavridis, *J. Chem. Phys.* **2002**, *116*, 9305–9314.
9. “On the ground states of CaC and ZnC: a multireference Brillouin-Wigner coupled cluster study.”, I. S. K. Kerkines, J. Pittner, P. Čársky, A. Mavridis and I. Hubač, *J. Chem. Phys.* **2002**, *117*, 9733–9739.
10. “Electronic structure and bonding nature of the ground state monocarbide cations,  $ScC^+$ ,  $TiC^+$ ,  $VC^+$ , and  $CrC^+$ .”, I. S. K. Kerkines and A. Mavridis, *Collect. Czech. Chem. Commun.* **2003**, *68*, 387–404 (invited paper on the occasion of the 60<sup>th</sup> birthday of Petr Čársky, Ivan Hubač and Miroslav Urban).
11. “Ab Initio Study of the Ground and Excited States of Zinc Carbide, ZnC.”, A. Tsouloucha, I. S. K. Kerkines and A. Mavridis, *J. Phys. Chem. A* **2003**, *107*, 6062–6072.
12. “Electronic Structure of Vanadium and Chromium Carbide Cations,  $VC^+$  and  $CrC^+$ . Ground and Low-Lying States.”, I. S. K. Kerkines and A. Mavridis, *Mol. Phys.* **2004**, *102*, 2451–2466 (invited paper in honor of Prof. Nicholas C. Handy).
13. “Theoretical Investigation of Organo-Noble Gas Compounds,  $HC(Ng)_n^+$ ,  $n = 1, 2$ ; Ng = He, Ne, Ar, Kr, and Xe. Evidence for Potentially Isolable  $HCAr_n^+$ ,  $HCKr_n^+$ , and  $HCXe_n^+$  Species.”, A. Papakondylis, I. S. K. Kerkines, and A. Mavridis, *J. Phys. Chem. A* **2004**, *108*, 11127–11131.

14. “Ground states of BeC and MgC: a comparative multireference Brillouin-Wigner coupled cluster and configuration interaction study.”, V. I. Teberekidis, I. S. K. Kerkines, C. A. Tsipis, P. Čársky, and A. Mavridis, *Int. J. Quantum Chem.* **2005**, *102*, 762–774 (invited paper for the special issue in memory of John Pople).
15. “On the electron affinity of SiN and spectroscopic constants of SiN”, I. S. K. Kerkines and A. Mavridis, *J. Chem. Phys.* **2005**, *123*, 124301–6.
16. “A Multireference Coupled-Cluster Potential Energy Surface of Diazomethane, CH<sub>2</sub>N<sub>2</sub>”, I. S. K. Kerkines, P. Čársky, and A. Mavridis, *J. Phys. Chem. A* **2005** *109*, 10148–10152.
17. “Structure and Energetics of Gaseous HZnCl”, I. S. K. Kerkines, A. Mavridis and P. A. Karipidis, *J. Phys. Chem. A* **2006**, *110*, 10899–10903.
18. “A Theoretical Study of Calcium Monohydride, CaH: Low-Lying States and Their Permanent Dipole Moments”, I. S. K. Kerkines and A. Mavridis, *J. Phys. Chem. A* **2007**, *111*, 371–374.
19. “Progress in ISOL target-ion-source-systems”, U. Köster, O. Arndt, E. Bouquerel, V. N. Fedoseyev, H. Frånberg, A. Joinet, C. Jost, I. S. K. Kerkines, R. Kirchner, and the TARGISOL Collaboration, *Nucl. Instr. and Meth. in Phys. Res. B*, **2008**, *266*, 4229–4239.
20. “Photodissociation of ClN<sub>3</sub> at 157 nm: Theory suggests a pathway leading to cyclic-N<sub>3</sub>.”, I. S. K. Kerkines, Z. Wang, P. Zhang, and K. Morokuma, *J. Chem. Phys.* **2008**, *129*, 171101–5.
21. “Analytical potential energy surfaces for N<sub>3</sub> low-lying doublet states”, Z. Wang, I. S. K. Kerkines, K. Morokuma, and P. Zhang, *J. Chem. Phys.* **2009**, *130*, 044313–18.

22. “Emitting and electron-transfer electronic states of tertiary amine-fluorophore sensor systems”, I. D. Petsalakis, I. S. K. Kerkines, N. N. Lathiotakis, and G. Theodorakopoulos, *Chem. Phys. Lett.* **2009**, *474*, 278–284.
23. “Structures and energies of low-lying doublet excited states of  $N_3$  from accurate configuration interaction calculations”, I. S. K. Kerkines, Z. Wang, P. Zhang, and K. Morokuma, *Mol. Phys.* **2009**, *107*, 1017–1025 (H. F. Schaefer III *Festschrift*).
24. “Low-lying absorption and emission spectra of pyrene, 1,6-dithiapyrene, and tetrathiafulvalene: A comparison between ab initio and time-dependent density functional methods”, I. S. K. Kerkines, I. D. Petsalakis, G. Theodorakopoulos, and W. Klopper, *J. Chem. Phys.* **2009**, *131*, 224315–10.
25. “Experimental and theoretical study of the reaction of  $POCl_3^-$  with  $O_2$ ”, I. S. K. Kerkines, K. Morokuma, N. Iordanova, and A. A. Viggiano, *J. Chem. Phys.* **2010**, *132*, 044309–9.
26. “Li atoms attached to helium nanodroplets”, A. Hernando, R. Mayol, M. Pi, M. Barranco, I. S. K. Kerkines, and A. Mavridis, *Int. J. Quantum Chem.*, **2011**, *111*, 400–5.
27. “Excited state intramolecular proton transfer in hydroxy oxime-based chemical sensors”, I. S. K. Kerkines, I. D. Petsalakis, G. Theodorakopoulos, and J. Rebek, Jr., *J. Phys. Chem. A* **2011**, *115*, 834–840.
28. “Theoretical study on the electronic structure and the absorption spectra of complexes of  $C_{60}$  and  $C_{59}N$  with  $\pi$ -extended derivatives of tetrathiafulvalene”, I. D. Petsalakis, D. Tzeli, I. S. K. Kerkines, and G. Theodorakopoulos, *Comput. Theor. Chem.* **2011**, *965*, 168–175.

29. “Fluorescence properties of organic dyes: Quantum chemical studies on the green/blue neutral and protonated DMA-DPH emitters in polymer matrices”, I. S. K. Kerkines, I. D. Petsalakis, P. Argitis, and G. Theodorakopoulos, *Phys. Chem. Chem. Phys.*, **2011**, *13*, 21273-21281.
30. “Short- and long-range binding of Be with Mg in the X  $^1\Sigma^+$  ground state and in the A  $^1\Pi$  excited state”, I. S. K. Kerkines and C. A. Nicolaides, *J. Chem. Phys.* **2012**, *137*, 124309.

#### **E. Publications in greek journals**

31. “The Story of the Discovery of Noble Gases and their Compounds.”, I. S. Kerkines, *Chemica Cronica (General Ed.)* **1997**, *7-8*, 207–210.
32. “The Contribution of Greece and Egypt to the Birth of Alchemy.”, I. S. Kerkines, *Panaegyptia*, **1999**, *86*, 23.
33. “Chemistry on the Internet”, I. S. Kerkines, *Chemica Cronica (General Ed.)* **2002**, *3*, 87–91.
34. “Chemical War Compounds”, S. G. Marinakis and I. S. Kerkines, *Stratitotiki Epitheorisi (Military Review)*, **2002**, *5*, 106-121.