

Dr. Ioannis Kerkinis

Publication list

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1. “Ab Initio Investigation of the LiHe X $^2\Sigma^+$, A $^2\Pi$ and B $^2\Sigma^+$ States. A Basis Set Study.”, I. S. K. Kerkinis and A. Mavridis, *J. Phys. Chem. A* **2000**, *104*, 408–412.
2. “Electronic Structure of Scandium and Titanium Carbide Cations, ScC⁺ and TiC⁺. Ground and Low-Lying States.”, I. S. K. Kerkinis and A. Mavridis, *J. Phys. Chem. A* **2000**, *104*, 11777–11785.
3. “An Accurate Description of the LiNe X $^2\Sigma^+$, A $^2\Pi$ and B $^2\Sigma^+$ States.”, I. S. K. Kerkinis and A. Mavridis, *J. Phys. Chem. A* **2001**, *105*, 1983–1987.
4. “On the Bonding Nature of the N₅⁺(= N(N₂)₂⁺) Cation and Related Species, N(CO)_x⁺, N(NH₃)_x⁺, and NR_x⁺, x = 1, 2; R = He, Ne, Ar, Kr. Do We Really Need the Resonance Concept?”, I. S. K. Kerkinis, A. Papakondylis, and A. Mavridis, *J. Phys. Chem. A* **2002**, *106*, 4435–4442.
5. “Theoretical Investigation of the X $^2\Sigma^+$, A $^2\Pi$ and B $^2\Sigma^+$ States of LiAr and LiKr.”, I. S. K. Kerkinis and A. Mavridis, *J. Chem. Phys.* **2002**, *116*, 9305–9314.
6. “On the ground states of CaC and ZnC: a multireference Brillouin-Wigner coupled cluster study.”, I. S. K. Kerkinis, J. Pittner, P. Čársky, A. Mavridis and I. Hubač, *J. Chem. Phys.* **2002**, *117*, 9733–9739.
7. “Electronic structure and bonding nature of the ground state monocarbide cations, ScC⁺, TiC⁺, VC⁺, and CrC⁺.”, I. S. K. Kerkinis and A. Mavridis, *Collect. Czech. Chem. Commun.* **2003**, *68*, 387–404 (invited paper on the occasion of the 60th birthday of Petr Čársky, Ivan Hubač and Miroslav Urban).

8. “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.
9. “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).
10. “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.
11. “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).
12. “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.
13. “A Multireference Coupled-Cluster Potential Energy Surface of Diazomethane, CH₂N₂”, I. S. K. Kerkines, P. Čársky, and A. Mavridis, *J. Phys. Chem. A* **2005** *109*, 10148–10152.
14. “Structure and Energetics of Gaseous HZnCl”, I. S. K. Kerkines, A. Mavridis and P. A. Karipidis, *J. Phys. Chem. A* **2006**, *110*, 10899–10903.
15. “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.

16. “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.
17. “Photodissociation of ClN_3 at 157 nm: Theory suggests a pathway leading to cyclic- N_3 .”, I. S. K. Kerkines, Z. Wang, P. Zhang, and K. Morokuma, *J. Chem. Phys.* **2008**, *129*, 171101–5.
18. “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**, *in press*. (H. F. Schaefer III *Festschrift*)
19. “Analytical potential energy surfaces for N_3 low-lying doublet states”, Z. Wang, I. S. K. Kerkines, K. Morokuma, and P. Zhang, *J. Chem. Phys.* **2009**, *in press*.
20. “Multireference Configuration Interaction and Coupled Cluster Calculations and Their Applications to Metal Carbides: Results from a Distributed Method and Program Development Project”, I. S. K. Kerkines, A. Mavridis, J. Pittner, and P. Čársky, *J. Comput. Chem.*, *submitted for publication*.

(Publications in Greek):

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