Εργαστήριο Φυσικοχημείας

Δημοσιεύσεις 2001-2005

Γ. Ερευνητικές εργασίες
Research papers

1. A. Kelarakis, V. Havredaki, K. Viras, W. Mingvanish, F. Heatley, C. Booth, and S.-M. Mai
Aqueous solutions and gels of diblock copolymers of 1,2-butylene oxide and ethylene oxide studied by light scattering and rheology
J. Phys. Chem. B, **105**, 7384 (2001)

2. A. Kelarakis, V. Havredaki, C. J. Rekatas, S.-M. Mai, D. Attwood, C. Booth, A. J. Ryan, I. W. Hamley, L. G. A. Martini
Association properties of a diblock copolymer of ethylene oxide and styrene oxide in aqueous solution studied by light scattering and rheometry
Macromol. Chem. Physic., **202**, 1345 (2001)

3. A. Kelarakis, S.-M. Mai, V. Havredaki, V. M. Nace and C. Booth
Effect of end group on the micelle properties of diblock copolymers of ethylene oxide and 1,2-butylene oxide
Phys. Chem. Chem. Phys., **3**, 4037 (2001)

4. A. Kelarakis, V. Castelletto, C. Chaibundit, J. Fundin, V. Havredaki, I. W. Hamley, and C. Booth
Rheology and structures of aqueous gels of triblock(oxyethylene/oxybutylene/oxyethylene) copolymers with lengthy oxyethylene blocks
Langmuir, **17**, 4232 (2001)

5. A. Kelarakis, V. Havredaki, C. J. Rekatas and C. Booth
Thermodynamics of micellisation of a diblock copolymer of ethylene oxide and styrene oxide in water
Phys. Chem. Chem. Phys., **3**, 5550 (2001)

6. A. D. Koutselos
Third-order transport properties of ions in electrostatic fields
Chem. Phys., **270**, 165 (2001)

7. J. C. Papaioannou, N. D. Papadimitropoulos and K. Viras
Dielectric behaviour of alpha-cyclodextrin, heptakis (2,3,6-tri-O-methyl)-beta-cyclodextrin, randomly methylated beta-cyclodextrin and low frequency Raman spectra of alpha- and beta-cyclodextrins
Mol. Phys., **99**, 239 (2001)

8. C. Tsonos, L. Apekis, K. Viras, L. Stepanenko, L. Karabanova, L. Sergeeva
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Solid State Ionics, **143**, 229 (2001)

9. A. S. Vatalis, A. Kanapitsas, C. G. Delides, K. Viras, P. Pissis
Phase behavior and molecular mobility in polyurethane/styrene-acrylonitrile blends
J. Appl. Polym. Sci., **80**, 1071 (2001)

10. G. Chatzis, J. Samios
CCl_4: A molecular dynamics study
J. Phys. Chem. A, **105**, 9522 (2001)

11. I. E. Molinou, N. G. Tsierkezos
Conductance studies on manganese(II), cobalt(II), nickel(II), and cadmium(II) sulfates in water + N,N-dimethylformamide mixtures at 293.15 K
J. Chem. Eng. Data, **46**, 1399 (2001)

12. D. P. Pullman, A. A. Tsekouras, Y. L. Li, J. J. Yang, M. R. Tate, D. B. Gosalvez, K. B. Laughlin, M. T. Schulberg, and S. T. Ceyer
Reactivity of Fluorinated Si(100) with F_2
J. Phys. Chem. B, **105**, 486 (2001)

13. A. Kalemos, A. Mavridis, and J. F. Harrison
Theoretical investigation of scandium carbide, ScC
J. Phys. Chem. A, **105**, 755 (2001)

14. D. Tzeli and A. Mavridis
First principles investigation of boron and aluminum carbides, BC, AlC and their anions, BC^- and AlC^-. 1
J. Phys. Chem. A, **105**, 1175 (2001)

15. I. S. K. Kerkines and A. Mavridis
An accurate description of the LiNe X $^2\Sigma^+$, A $^2\Pi$, and B $^2\Sigma^+$ States
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16. A. Papakondylis and A. Mavridis
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19. D.Tzeli, A. Mavridis and S. Xantheas
A molecular level study of the aqueous microsolvation of acetylene
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Macromolecules, **35**, 5591 (2002)

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Low-frequency Raman spectroscopy of n-alcohols. LAM vibration and crystal structure
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23. M. Chalaris, J. Samios
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Z. Phys. Chem., **216**, 961 (2002)

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Relative permittivities, speeds of sound, viscosities, and densities of cyclohexanone + *cis*-decalin and cyclohexanone + *trans*-decalin mixtures at 283.15, 293.15, and 303.15 K
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28. H. S. Karayianni, G. S. Patermarakis, J. C. Papaioannou
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29. T. C. Ghikas, J. C. Papaioannou
Dielectric relaxation of α-cyclodextrin-polyiodide complexes (α-cyclodextrin)$_2 \cdot LiI_3 \cdot I_2 \cdot 8H_2O$ and (α-cyclodextrin)$_2 \cdot Cd_{0.5} \cdot I_5 \cdot 26H_2O$
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Dielectric relaxation of the beta-cyclodextrin complexes with tridecanoic acid and 1,13-tridecanedioic acid
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Theoretical investigation of titanium carbide, TiC: $X^3\Sigma^+$, $a^1\Sigma^+$, $A^3\Delta$, and $b^1\Delta$ States
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Theoretical investigation of iron carbide, FeC
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An accurate description of the ground and excited states of SiH
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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 and R = He, Ne, Ar, Kr. Do we really need the resonance concept?
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First principles examination of the acetylene-water clusters, HCCH-$(H_2O)_x$, x = 2, 3, and 4
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On the ground states of CaC and ZnC: A multireference Brillouin-Wigner coupled cluster study
J. Chem. Phys., **117**, 9733 (2002)

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Micellization and gelation of triblock copolymers of ethylene oxide and styrene oxide in aqueous solution
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Chain Folding in Semicrystalline Oxybutylene/Oxyethylene/Oxybutylene Triblock Copolymers Studied by Raman Spectroscopy
J. Phys. Chem. B., **107**, 6946 (2003)

41. A. Kelarakis, V. Havredaki, X.-F. Yuan, Y.-W. Yang, and C. Booth
Mixed micelles of block copolymers of ethylene oxide and 1,2-butylene oxide. Solutions and gels of triblock BEB plus diblock EB copolymers studied by light scattering and rheology
J. Mater. Chem., **13**, 2779 (2003)

42. G. Balla and A. D. Koutselos
Molecular dynamics simulation of ion transport in moderately dense gases in an electrostatic field
J. Chem. Phys., **119**, 11374 (2003)

43. D. Fragiadakis, M. Bouga, A. Kyritsis, P. Pissis, K. Viras, W. Mingvanish, C. Booth
Molecular order and dynamics in block copolymers of poly(oxybutylene) and poly(oxyethylene)
Macromol. Symp., **191**, 21 (2003)

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Binary mixtures of supercritical carbon dioxide with methanol. A molecular dynamics simulation study
Chem. Phys. Lett., **374**, 187 (2003)

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Conductivities, Partial Molar Volumes, and Isentropic Compressibilities of Sodium, Potassium and Ammonium Thiocyanates in Water + N,N-Dimethylformamide Mixtures at 20°C
Z. Phys. Chem., **217**, 1075 (2003)

46. J. C. Papaioannou, T. C. Ghikas
Dielectric relaxation of α-cyclodextrin-polyiodide complexes (α-cyclodextrin)$_2$ · BaI_2 · I_2 · 8H_2O and (α-cyclodextrin)$_2$ · KI_3 · I_2 · 8H_2O
Mol. Phys., **101**, 2601 (2003)

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On the dipole moment of the ground state X $^3\Delta$ of iron carbide, FeC
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Electronic structure and bonding nature of the ground state monocarbide cations ScC^+, TiC^+, VC^+, and CrC^+
Collect. Czech. Chem. Commun., **68**, 387 (2003) [invited article]

49. A. Kalemos, T. H. Dunning, Jr., J. F. Harrison, and A. Mavridis
Electronic structure of linear TiCH
J. Chem. Phys., **119**, 3745 (2003)

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Ab inition study of the ground and excited states of zinc carbide, ZnC
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51. A. Metropoulos, A. Papakondylis and A. Mavridis
Ab initio investigation of the ground state properties of PO, PO^+ and PO^-
J. Chem. Phys., **119**, 5981 (2003)

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Theoretical investigation of the electronic states of calcium carbide, CaC
J. Phys. Chem. A, **107**, 7650 (2003)

53. A. Kalemos, T. H. Dunning, Jr. and A. Mavridis
On the symmetry breaking of BNB. Real or artifactual?
J. Chem. Phys., **120**, 1813 (2004)

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On the ground state of the titanium phospide, TiP. A theoretical investigation
J. Chem. Phys., **121**, 2646 (2004)

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Electronic structure of vanadium and chromium carbide cations, VC^+ and CrC^+. Ground and low-lying states
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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
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The electronic structure of vanadium carbide, VC
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