

Curriculum vitae

Dr. Heribert Reis

Date of birth: 12.10.1961 in Solingen, Germany

Nationality: German

Marital status: single

Academic career:

- 1981-1987 Study of Chemistry at the Johannes-Gutenberg-Universitaet Mainz, Germany
- 1987-1988 Diploma with Prof. Baumann at the Department of Physical Chemistry, title: "Computer-aided recording of electrooptical spectra; spectroscopic investigations on p,p'-disubstituted diphenyl-acetylen derivatives", grade "sehr gut" (very good)
- 1988-1995 Ph.D. with Prof. Baumann, subject: "Influence of rotational diffusion on the electric field induced effect on the fluorescence spectra of diluted solutions" (Determination of dipole moments of organic molecules in electronically excited states), grade "Magna cum laude".
- March-July 1990 Stay with Prof. Bek at the "Instituto Químico de Sarrià" in Barcelona/Spain.
- 1995-1997 Scientific employee at the Department of Physical Chemistry at the university of Mainz
- Nov. 1996 - Stay at the Departamento the Química Orgánica of the University of Havana/Cuba, giving a lecture "Introducción a la fotoquímica".
- Feb. 1997 - Participation at the TMR project "Delos" as a postdoc, working with Dr. Manthos Papadopoulos, Institute of Pharmaceutical and Organic Chemistry, National Hellenic Research Foundation, Athens, Greece.
- March 1997 -
- May 2000 "Development and applications of methods for the calculation of the macroscopic linear and nonlinear susceptibilities in crystals"
- May 2000- Sept 2005 Participation in several projects at the National Hellenic Research Foundation
- Since Sept. 2005 Researcher at the National Hellenic Research Foundation, Athens, Greece.

Publications:

1. S.V. Rodrigues, A.K. Maiti, H. Reis, W. Baumann, "Electrooptical Emission Measurements on a Nonconjugated Bichromophoric Donor-Acceptor Molecule", MOLECULAR PHYSICS 1992, Vol 75, pp 953-960.

2. W. Baumann, Z. Nagy, H. Reis, N. Detzer,
“Electric-Field-Induced Anisotropy Spectra”,
CHEMICAL PHYSICS LETTERS 1994, Vol 224, pp 517-524.
3. N.A. Nemkovich, W. Baumann, H. Reis, N. Detzer,
“Dipole-Moments of Aminophthalimides Determined by Modified Electrooptical
Absorption and Emission Measurements”,
JOURNAL OF PHOTOCHEMISTRY AND PHOTOBIOLOGY A-CHEMISTRY
1995, Vol 89, pp 127-133.
4. N.A. Nemkovich, W. Baumann, H. Reis, Y.V. Zvinevich,
“Electrooptical and Laser Spectrofluorometry Study of Coumarin-7 and Coumarin-30
- Evidence for the Existence of the Close-Lying Electronic States and Conformers”,
JOURNAL OF PHOTOCHEMISTRY AND PHOTOBIOLOGY A-CHEMISTRY
1997, Vol 109, pp 287-292.
5. N.A. Nemkovich, H. Reis, W. Baumann,
“Ground and Excited-State Dipole-Moments of Coumarin Laser-Dyes - Investigation
by Electrooptical Absorption and Emission Methods”,
JOURNAL OF LUMINESCENCE 1997, Vol 71, pp 255-263.
6. C. Carvalho, I. Brinn, W. Baumann, H. Reis, Z. Nagy,
“Excited-State Acidity of Bifunctional Compounds .5. 5-(2-Hydroxyphenyl)-3-
Phenyl-1,2,4-Oxadiazole and 3-(2-Hydroxyphenyl)-5-Phenyl-1,2,4-Oxadiazole”,
JOURNAL OF THE CHEMICAL SOCIETY-FARADAY TRANSACTIONS 1997,
Vol 93, pp 3325-3329.
7. H. Reis, W. Baumann,
“Influence of Rotational Diffusion on the Electric-Field-Induced Effect on the
Fluorescence-Spectrum of Diluted Solutions .1. Theory and Numerical Simulations”,
CHEMICAL PHYSICS 1997, Vol 214, pp 383-407.
8. K. Nishiyama, T. Honda, H. Reis, U. Mueller, K. Muellen, W. Baumann,
T. Okada,
“Electronic-Structures of 9,10-Anthrylene Dimers and Trimers in Solution -
Formation of Charge Separation States Depending on Alkyl Substituent Groups”,
JOURNAL OF PHYSICAL CHEMISTRY A 1998, Vol 102, pp 2934-2943.
9. H. Reis, S. Raptis, M.G. Papadopoulos, R.H.C. Janssen, D.N. Theodorou, R.W.
Munn,
“Calculation of Macroscopic First-Order and 3rd-Order Optical Susceptibilities for
the Benzene Crystal”,
THEORETICAL CHEMISTRY ACCOUNTS 1998, Vol 99, pp 384-390.
10. H. Reis, M.G. Papadopoulos, R.W. Munn,

- “Calculation of Macroscopic First-Order, 2nd-Order, and 3rd-Order Optical Susceptibilities for the Urea Crystal”,
JOURNAL OF CHEMICAL PHYSICS 1998, Vol 109, pp 6828-6838.
11. N.A. Nemkovich, W. Baumann, H. Reis, Y.V. Zvinevich, A.N. Rubinov,
“Dipole-Moments of Laser Coumarins in the Ground and Excited Electronic States”,
OPTICS AND SPECTROSCOPY 1999, Vol 87, pp 735-741.
 12. R. Wortmann, S. Lebus, H. Reis, A. Grabowska, K. Kownacki, S. Jarosz,
“Spectral and Electrooptical Absorption and Emission Studies on Internally
Hydrogen-Bonded Benzoxazole Double Derivatives - 2,5-
bis(Benzoxazolyl)Hydroquinone (Bbhq) and 3,6-bis(Benzoxazolyl)Pyrocatechol
(Bbpc) - Single Versus Double Proton-Transfer in the Excited Bbpc Revisited”,
CHEMICAL PHYSICS 1999, Vol 243, pp 295-304.
 13. H. Reis, M.G. Papadopoulos,
“Nonlinear-Optical Properties of the Rhombic B₄-Cluster”,
JOURNAL OF COMPUTATIONAL CHEMISTRY 1999, Vol 20, pp 679-687.
 14. H. Reis, M.G. Papadopoulos, I. Boustani, “DFT calculations of Static Dipole
Polarizabilities and Hyperpolarizabilities for the Boron Clusters B_n (n=3-8,10)”,
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY 2000, Vol 78, pp
131-135.
 15. H. Reis, M.G. Papadopoulos, C. Haettig, J.G. Angyan, R.W. Munn
“Distributed First and 2nd-Order Hyperpolarizabilities - An Improved Calculation of
Nonlinear-Optical Susceptibilities of Molecular Crystals”,
JOURNAL OF CHEMICAL PHYSICS 2000, Vol 112, pp 6161-6172.
 16. H. Reis, M.G. Papadopoulos, P. Calaminici, K. Jug, A. Köster,
“Calculation of macroscopic linear and nonlinear optical
susceptibilities for the naphthalene, anthracene and meta-nitroaniline crystals”,
CHEMICAL PHYSICS 2000, Vol 261, pp 359-371.
 17. H. Reis, S.G. Raptis, M.G. Papadopoulos,
“Electrostatic calculation of linear and nonlinear optical properties of ice Ih, II, IX
and VIII.”,
CHEMICAL PHYSICS 2001, Vol. 263, 301-16.
 18. A. Detsi, E. Gavrielatos, M.A. Adam, O. Igglessi-Markopoulou, J. Markopoulos, M.
Theologitis, H. Reis and M.G. Papadopoulos,
“Synthesis of N-Urethane-Protected Gamma-Amino-Functionalized Butenoates and
Tautomeric Studies by Means of NMR, X-Ray Crystallography and Ab-Initio
Calculations”, EUROPEAN JOURNAL OF ORGANIC CHEMISTRY 2001, pp
4337-4342

19. H. Reis, M.G. Papadopoulos, D.N. Theodorou,
“Calculation of Refractive-Indexes and 3rd-Harmonic Generation Susceptibilities of Liquid Benzene and Water - Comparison of Continuum and Discrete Local-Field Theories”, JOURNAL OF CHEMICAL PHYSICS 2001, Vol 114, pp 876-881.
20. H Reis, S. Raptis, M.G. Papadopoulos,
“Comparison of the non-linear optical properties of a dimethylaminostilbene derivative containing a molybdenum mononitrosyl redox centre and of p,p'-dimethylaminonitrostilbene calculated by ab-initio methods”, PHYSICAL CHEMISTRY CHEMICAL PHYSICS 2001, Vol. 3, 3901-3905
21. R.W. Munn, M.G. Papadopoulos, H. Reis,
“Local fields and distributed response: Electric susceptibility calculations for molecular materials”, POLISH JOURNAL OF CHEMISTRY 2002, Vol. 76, 155-165.
22. H Reis, M.G. Papadopoulos,
“Calculation of the first hyperpolarizabilities of the neutral and the cationic form of a donor-acceptor molecule containing octamethylferrocene”, PHYSICAL CHEMISTRY CHEMICAL PHYSICS 2003, Vol. 5, 1190-1192.
23. H. Reis, M. G. Papadopoulos, A. Avramopoulos,
“Calculation of the microscopic and macroscopic linear and nonlinear optical properties of acetonitrile: I. Accurate molecular properties in the gas phase and susceptibilities of the liquid in Onsager's reaction-field model”, JOURNAL OF PHYSICAL CHEMISTRY A 107, 3907-3917, 2003.
24. R. Wortmann, S. Lebus-Henn, H. Reis, M. G. Papadopoulos,
“[Off-diagonal second-order polarizability of N,N'-dihexyl-1,3-diamino-4,6-dinitrobenzene](#)”,
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM 633 (2-3): 217-226, 2003
25. H Reis, M. Makowska-Janusika, M. G. Papadopoulos,
“[Nonlinear optical susceptibilities of poled guest-host systems: A computational approach](#)”
JOURNAL OF PHYSICAL CHEMISTRY B 108 (26): 8931-8940, 2004
26. Avramopoulos A, Reis H, Li JB, et al.
“[The dipole moment, polarizabilities, and first hyperpolarizabilities of HArF. A computational and comparative study](#)”
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY 126 (19): 6179-6184, 2004

27. Makowska-Janusik M, Reis H, Papadopoulos MG, et al.
Molecular dynamics simulations of electric field poled nonlinear optical chromophores incorporated in a polymer matrix
JOURNAL OF PHYSICAL CHEMISTRY B 108 (2): 588-596, 2004
28. Papadopoulos MG, Reis H, Avramopoulos A, et al.
A comparative study of the dipole polarizability of some Zn clusters
J PHYS CHEM B 109 (40): 18822-18830 OCT 13 2005
28. Makowska-Janusik M, Reis H, Papadopoulos MG, Economou IG
Peculiarities of electric field alignment of nonlinear optical chromophores incorporated into thin film polymer matrix.
THEORETICAL CHEMISTRY ACCOUNTS 114 (1-3): 153-158 SEP 2005
30. Souli C, Avlonitis N, Calogeropoulou T, Tsoinias A, Maksay G, Biro T, Politi A, Mavromoustakos T, Makriyannis A, Reis H, Papadopoulos M
Novel 17 beta-substituted conformationally constrained neurosteroids that modulate GABA(A) receptors
JOURNAL OF MEDICINAL CHEMISTRY 48 (16): 5203-5214 AUG 11 2005
31. H. Reis, A. Grzybowski, and M. G. Papadopoulos
Computer Simulation of the Linear and Nonlinear Optical Susceptibilities of *p*-Nitroaniline in Cyclohexane, 1,4-Dioxane, and Tetrahydrofuran in Quadrupolar Approximation. I. Molecular Polarizabilities and Hyperpolarizabilities
JOURNAL OF PHYSICAL CHEMISTRY A 109, 9911, 2005
32. Munn, RW; Papadopoulos, MG; Reis, H
Local fields and distributed response: Electric susceptibility calculations for molecular materials
POLISH JOURNAL OF CHEMISTRY 76 (2002) 155-165
32. Alparone, A; Reis, H; Papadopoulos, MG
Theoretical investigation of the (hyper) polarizabilities of pyrrole homologues C₄H₄XH (X = N, P, As, Sb, Bi). A coupled-cluster and density functional theory study
JOURNAL OF PHYSICAL CHEMISTRY A 110 (2006) 5909-5918
33. Papadopoulos, MG; Reis, H; Avramopoulos, A; Erkoc, S; Amirouche, L
Polarizabilities and second hyperpolarizabilities of ZnM₂C₄N clusters
MOLECULAR PHYSICS 104 (2006) 2027-2036
34. Reis, H; Papadopoulos, MG; Grzybowski, A
Computer simulation of the linear and nonlinear optical susceptibilities of *p*-nitroaniline in cyclohexane, 1,4-dioxane, and tetrahydrofuran in quadrupolar approximation. II. Local field effects and optical susceptibilities
JOURNAL OF PHYSICAL CHEMISTRY B 125 (2006) 18537-18552

35. Reis, H
Problems in the comparison of theoretical and experimental hyperpolarizabilities revisited
JOURNAL OF CHEMICAL PHYSICS 125 (2006) 014506
36. Avramopoulos, A; Papadopoulos, MG; Reis, H
Calculation of the microscopic and macroscopic linear and nonlinear optical properties of liquid acetonitrile. II. Local fields and linear and nonlinear susceptibilities in quadrupolar approximation
JOURNAL OF PHYSICAL CHEMISTRY B 111 (2007) 2546-2553.
37. Avramopoulos, A; Serrano-Andres, L; Li, JB; Reis, H; Papadopoulos, MG
Linear and nonlinear optical properties of some organoxenon derivatives
JOURNAL OF CHEMICAL PHYSICS 127 (2009) 214102
38. Durdagi, S; Reis, H; Papadopoulos, MG; Mavromoustakos, T
Comparative molecular dynamics simulations of the potent synthetic classical cannabinoid ligand AMG3 in solution and at binding site of the CB1 and CB2 receptors
BIOORGANIC & MEDICINAL CHEMISTRY 16 (2008) 7377-7388
39. Loboda, O; Zalesny, R; Avramopoulos, A; Luis, JM; Kirtman, B; Tagmatarchis, N; Reis, H; Papadopoulos, MG
JOURNAL OF PHYSICAL CHEMISTRY A 113 (2009) 1159-1170
40. Luis, JM; Reis, H; Papadopoulos, M; Kirtman, B
Treatment of nonlinear optical properties due to large amplitude anharmonic vibrational motions: Umbrella motion in NH₃
JOURNAL OF CHEMICAL PHYSICS 131 (2009) 034116