

## Publikacje naukowe w czasopismach międzynarodowych

Wykaz zawiera publikacje naukowe w czasopismach o zasięgu międzynarodowym dokumentowane w Politechnice Wrocławskiej za lata 1994–2014, w których co najmniej jeden z autorów posiadał afiliację w Instytucie Chemii Fizycznej i Teoretycznej. W obrębie każdego roku wprowadzono układ alfabetyczny wg pierwszego autora.

### 2014

1. Adach A., Daszkiewicz M., Golonka M., Misiaszek T., Grabka D.: *In situ synthesis of scorpion-like complexes isolated from the system containing zerovalent nickel*. Polyhedron. 2014, Vol. 78, s. 31–39.
2. Bąkowiec J.B., Olejarz J., Turowska-Tyrk I.: *Steering photochemical reactivity of 2,4,6-triisopropylbenzophenonate anion in a crystalline state*. Journal of Photochemistry and Photobiology. A. 2014, Vol. 273, s. 34–42.
3. Bąkowiec J.B., Turowska-Tyrk I.: *Structural transformations in crystals induced by radiation and pressure. Pt. 1, How pressure influences the intramolecular photochemical reactions in crystals*. CrystEngComm. 2014, Vol. 16, No. 27, s. 6039–6048.
4. Bazylińska U.J., Drozdek S., Nyk M.W., Kulbacka J., Samoć M., Wilk K.: *Core/shell quantum dots encapsulated in biocompatible oil-core nanocarriers as two-photon fluorescent markers for bioimaging*. Langmuir. 2014, Vol. 30, No. 49, s. 14931–14943.
5. Camposeo A., Del Carro P., Persano L., Cyprych K.M., Szukalski A., Sznitko L., Myśliwiec J., Pisignano D.: *Physically transient photonics: random versus distributed feedback lasing based on nanoimprinted DNA*. ACS Nano. 2014, Vol. 8, No. 10, s. 10893–10898.
6. Choi E.Y., Mazur L.M., Mager L., Gwon M., Pitrat D., Mulatier J.C., Monnereau C., Fort A., Attias A., Dorkenoo, Kwon J.E., Xiao Y., Matczyszyn K., Samoć M.,

- Kim D.W., Nakao A., Heinrich B., Hashizume D., Uchiyama M., Park S.Y., Mathevet F., Aoyama T., Andraud C., Wu J.W., Barsella A., Ribierre J.-C.: *Photophysical, amplified spontaneous emission and charge transport properties of oligofluorene derivatives in thin films*. *Physical Chemistry Chemical Physics*. 2014, Vol. 16, No. 32, s. 16941–16956.
7. Cichy B., Wawrzyńczyk D.M., Bednarkiewicz A., Samoć M., Stręk W.: *Optical nonlinearities and two-photon excited time-resolved luminescence in colloidal quantum-confined CuInS<sub>2</sub>/ZnS heterostructures*. *RSC Advances*. 2014, Vol. 4, No. 64, s. 34065–34072.
  8. Cioslowski J., Strasburger K., Matito E.: *Benchmark calculations on the lowest-energy singlet, triplet, and quintet states of the four-electron harmonium atom*. *Journal of Chemical Physics*. 2014, Vol. 141, No. 4, art. 044128, s. 1–6.
  9. Cyprych K.M., Sznitko L., Myśliwiec J.: *Starch: application of biopolymer in random lasing*. *Organic Electronics*. 2014, Vol. 15, No. 10, s. 2218–2222.
  10. Dradrach K., Bartkiewicz S., Miniewicz A.: *Electrooptical properties of hybrid liquid crystalline systems containing CdSe quantum dots*. *Applied Physics Letters*. 2014, Vol. 105, No. 23, art. 231903, s. 1–4.
  11. Dyguda-Kazimierowicz E.B., Roszak S., Sokalski A.: *Alkaline hydrolysis of organophosphorus pesticides: the dependence of the reaction mechanism on the incoming group conformation*. *Journal of Physical Chemistry B*. 2014, Vol. 118, No. 26, s. 7277–7289.
  12. Giedroyć-Piasecka W., Dyguda-Kazimierowicz E.B., Beker W.L., Mor M., Lodola A., Sokalski A.: *Physical nature of fatty acid amide hydrolase interactions with its inhibitors: testing a simple nonempirical scoring model*. *Journal of Physical Chemistry B*. 2014, Vol. 118, No. 51, s. 14727–14736.
  13. Gordel M., Olesiak-Bańska J., Kołkowski R., Matczyszyn K., Buckle M., Samoć M.: *Shell-thickness-dependent nonlinear optical properties of colloidal gold nanoshells*. *Journal of Materials Chemistry. C*. 2014, Vol. 2, No. 35, s. 7239–7246.
  14. Gordel M., Olesiak-Bańska J., Matczyszyn K., Nogues C., Buckle M., Samoć M.: *Post-synthesis reshaping of gold nanorods using a femtosecond laser*. *Physical Chemistry Chemical Physics*. 2014, Vol. 16, No. 1, s. 71–78.
  15. Grzelak J., Ciszak K., Nyk M.W., Maćkowski S., Piątkowski D.: *Extending light-harvesting of poly(3-hexylthiophene) through efficient energy transfer from infrared absorbing nanocrystals: single nanoparticle study*. *Applied Physics Letters*. 2014, Vol. 105, No. 16, art. 163114, s. 1–5.

16. Iwanejko J., Wojaczyńska E., Wojaczyński J., Bąkowicz J.B.: *Stereoselective preparation of chiral compounds in Mannich-type reactions of a bicyclic imine and phenols or indole*. Tetrahedron Letters. 2014, Vol. 55, No. 49, s. 6619–6622.
17. Jędrzejewska B., Krawczyk P., Gordel M., Samoć M.: *Synthesis and photophysical properties of two-photon chromophores containing 1H-benzimidazole residue*. Dyes and Pigments. 2014, Vol. 111, s. 162–175.
18. Karpiński P., Miniewicz A.: *Bidirectional molecular reorientation induced by localized surface plasmon*. RSC Advances. 2014, Vol. 4, No. 6, s. 2673–2677.
19. Kołkowski R., Samoć M.: *Modified Z-scan technique using focus-tunable lens*. Journal of Optics. 2014, Vol. 16, No. 12, art. 125202, s. 1–6.
20. Kołkowski R., Szeszko J., Dwir B., Kapon E., Zyss J.: *Effects of surface plasmon polariton-mediated interactions on second harmonic generation from assemblies of pyramidal metallic nano-cavities*. Optics Express. 2014, Vol. 22, No. 25, s. 30592–30606.
21. Kowalczyk R., Wierzba A., Boratyński P., Bąkowicz J.B.: *Enantioselective conjugate addition of aliphatic thiols to divergently activated electron poor alkenes and dienes*. Tetrahedron. 2014, Vol. 70, No. 35, s. 5834–5842.
22. Kozłowska J.J., Bartkowiak W.: *The effect of spatial confinement on the noble-gas HArF molecule: structure and electric properties*. Chemical Physics. 2014, Vol. 441, s. 83–92.
23. Kozłowska J.J., Zaleśny R., Bartkowiak W.: *On the nonlinear electrical properties of molecules in confined spaces – from cylindrical harmonic potential to carbon nanotube cages*. Chemical Physics. 2014, Vol. 428, s. 19–28.
24. Lipkowski P., Grabowski S.J.: *Could the lithium bond be classified as the  $\sigma$ -hole bond? – QTAIM and NBO analysis*. Chemical Physics Letters. 2014, Vol. 591, s. 113–118.
25. Lipkowski P., Kozłowska J.J., Roztoczyńska A.K., Bartkowiak W.: *Hydrogen-bonded complexes upon spatial confinement: structural and energetic aspects*. Physical Chemistry Chemical Physics. 2014, Vol. 16, No. 4, s. 1430–1440.
26. Lodowski P., Jaworska M., Andruniów T., Garabato B.D., Kozłowski P.M.: *Mechanism of Co-C bond photolysis in the base-on form of methylcobalamin*. Journal of Physical Chemistry A. 2014, Vol. 118, No. 50, s. 11718–11734.
27. Lodowski P., Jaworska M., Andruniów T., Garabato B.D., Kozłowski P.M.: *Mechanism of the S1 excited state internal conversion in vitamin B12*. Physical Chemistry Chemical Physics. 2014, Vol. 16, No. 35, s. 18675–18679.

28. Maliszewska I., Leśniewska A., Olesiak-Bańska J., Matczyszyn K., Samoć M.: *Biogenic gold nanoparticles enhance methylene blue-induced phototoxic effect on Staphylococcus epidermidis*. Journal of Nanoparticle Research. 2014, Vol. 16, No. 6, art. 2457, s. 1–16.
29. Masełko J., Kiehl M., Couture J., Dyonizy A., Kaminker V., Nowak P.M., Pantaleone J.: *Emergence of complex behavior in chemical cells: the system  $AlCl_3$ -NaOH*. Langmuir. 2014, Vol. 30, No. 20, s. 5726–5731.
30. Mazur L.M., Castiglione A., Ocytko K., Kameche F., Macabies R., Ainsebaa A., Kreher D., Heinrich B., Donnio B., Sanaur S., Lacaze E., Fave J.-L., Matczyszyn K., Samoć M., Weon W.J., Attias A.-J., Ribierre J.-C., Mathevet F.: *Charge carrier mobility study of a mesogenic thienothiophene derivative in bulk and thin films*. Organic Electronics. 2014, Vol. 15, No. 4, s. 943–953.
31. Miniewicz A., Girones J., Karpiński P., Mossety-Leszczak B., Galina H., Dutkiewicz M.: *Photochromic and nonlinear optical properties of azo-functionalized POSS nanoparticles dispersed in nematic liquid crystals*. Journal of Materials Chemistry. C. 2014, Vol. 2, No. 3, s. 432–440.
32. Misiaszek T., Czyżnikowska Ż.: *The nature of interactions in nicotinamide crystal*. Journal of Molecular Graphics & Modelling. 2014, Vol. 51, s. 73–78.
33. Morawski O., Sobolewski A.L., Kozankiewicz B., Sznitko L., Miniewicz A.: *On the origin of fluorescence emission in optically non-linear DCNP crystals*. Physical Chemistry Chemical Physics. 2014, Vol. 16, No. 48, s. 26887–26892.
34. Moreau J., Lux F., Four M., Olesiak-Bańska J., Matczyszyn K., Perriat P., Frochot C., Arnoux P., Tillement O., Samoć M., Ponterini G., Roux S., Lemercier G.: *A 5-(difluorenyl)-1,10-phenanthroline-based Ru(II) complex as a coating agent for potential multifunctional gold nanoparticles*. Physical Chemistry Chemical Physics. 2014, Vol. 16, No. 28, s. 14826–14833.
35. Murugan N.A., Zaleśny R., Kongsted J., Agren H.: *Chelation-induced quenching of two-photon absorption of azacrown ether substituted distyryl benzene for metal ion sensing*. Journal of Chemical Theory and Computation. 2014, Vol. 10, No. 2, s. 778–788.
36. Murugan N.A., Zaleśny R., Kongsted J., Nordberg A., Agren H.: *Promising two-photon probes for in vivo detection of  $\beta$  amyloid deposits*. Chemical Communications. 2014, Vol. 50, No. 79, s. 11694–11697.
37. Myśliwiec J., Szukalski A., Sznitko L., Miniewicz A., Haupa K., Żygadło K., Matczyszyn K., Olesiak-Bańska J., Samoć M.: *Synthesis, optical and nonlinear optical properties of new pyrazoline derivatives*. Dyes and Pigments. 2014, Vol. 102, s. 63–70.

38. Niezgoda I., Jaworska J., Kownacka M., Pociecha D., Galewski Z.: *Mesomorphic and trans-cis-trans photoisomerization studies of 4-[2-(4-hexyloxyphenyl)diazenyl]phenyl alkanoates*. Phase Transitions. 2014, Vol. 87, No. 10/11, s. 1038–1049.
39. Nyk M.W., Szeremeta J., Wawrzyńczyk D.M., Samoć M.: *Enhancement of two-photon absorption cross section in CdSe quantum rods*. Journal of Physical Chemistry C. 2014, Vol. 118, No. 31, s. 17914–17921.
40. Olech K., Sołoducho J., Laba K., Data P., Lapkowski M., Roszak S.: *The synthesis and characterization of -3,4-ethylenedioxythiophene derivatives with electroactive features*. Electrochimica Acta. 2014, Vol. 141, s. 349–356.
41. Panek J., Jezierska-Mazarello A., Lipkowski P., Martyniak A., Filarowski A.: *Comparison of resonance assisted and charge assisted effects in strengthening of hydrogen bonds in dipyrins*. Journal of Chemical Information and Modeling. 2014, Vol. 54, No. 1, s. 86–95.
42. Pawlik G., Miniewicz A., Sobolewska A.M., Mituś A.: *Generic stochastic Monte Carlo model of the photoinduced mass transport in azo-polymers and fine structure of surface relief gratings*. Europhysics Letters. 2014, Vol. 105, No. 2, art. 26002, s. p1–p6.
43. Pawlik G., Radosz W., Mituś A., Myśliwiec J., Miniewicz A., Kajzar F., Rau I.: *Holographic grating inscription in DRI: DNA-CTMA thin films: the puzzle of time scales*. Central European Journal of Chemistry. 2014, Vol. 12, No. 8, s. 886–892.
44. Puszyńska-Tuszkano M., Staszak Z., Misiaszek T., Klepka M.T., Wolska A., Drzewiecka-Antonik A., Fałtynowicz H., Golonka M.: *Metallophilic interactions in polynuclear Ag(I) complex with 1-methylhydantoin studied by X-ray absorption, electronic and vibrational spectroscopies*. Chemical Physics Letters. 2014, Vol. 597, s. 94–98.
45. Roszak R., Roszak S., Majumdar D., Firlej L., Kuchta B., Leszczynski J.: *Unique bonding nature of carbon-substituted Be<sub>2</sub> dimer inside the carbon (sp<sup>2</sup>) network*. Journal of Physical Chemistry A. 2014, Vol. 118, No. 30, s. 5727–5733.
46. Roztoczyńska A.K., Kozłowska J.J., Lipkowski P., Bartkowiak W.: *Does the spatial confinement influence the electric properties and cooperative effects of the hydrogen bonded systems? HCN chains as a case study*. Chemical Physics Letters. 2014, Vol. 608, s. 264–268.
47. Ryabchun A., Sobolewska A.M., Bobrovsky A., Shibaev V., Stumpe J.: *Polarization holographic grating recording in the cholesteric azobenzene-containing films with the phototunable helix pitch*. Journal of Polymer Science. Part B, Polymer Physics. 2014, Vol. 52, No. 11, s. 773–781.

48. Salomon A., Prior Y., Fedoruk M., Feldmann J., Kołkowski R., Zyss J.: *Plasmonic coupling between metallic nanocavities*. Journal of Optics. 2014, Vol. 16, No. 11, art. 114012, s. 1–7.
49. Schab-Balcerzak E., Konieczkowska J., Siwy M., Sobolewska A.M., Wójtowicz M., Wiącek M.: *Comparative studies of polyimides with covalently bonded azo-dyes with their supramolecular analogues: thermo-optical and photoinduced properties*. Optical Materials (Amsterdam). 2014, Vol. 36, No. 5, s. 892–902.
50. Schapiro I., Fusi S., Olivucci M., Andruniów T., Sasidharanpillai S., Loppnow G.R.: *Initial excited-state dynamics of an N-alkylated indanylidene-pyrroline (NAIP) rhodopsin analog*. Journal of Physical Chemistry B. 2014, Vol. 118, No. 42, s. 12243–12250.
51. Sobolewska A.M., Bartkiewicz S., Myśliwiec J., Singer K.D.: *Holographic memory devices based on a single-component phototropic liquid crystal*. Journal of Materials Chemistry. C. 2014, Vol. 2, No. 8, s. 1409–1412.
52. Sobolewska A.M., Bartkiewicz S., Priimagi A.: *High-modulation-depth surface relief gratings using s-s polarization configuration in supramolecular polymer-azobenzene complexes*. Journal of Physical Chemistry C. 2014, Vol. 118, No. 40, s. 23279–23284.
53. Sobolewska A.M., Noga J.E., Bartkiewicz S.: *Biphotonic photochromic reaction results in an increase in the efficiency of the holographic recording process in an azo polymer*. Langmuir. 2014, Vol. 30, No. 1, s. 17–21.
54. Sowula M., Misiaszek T., Bartkowiak W.: *Solvent effect on the vibrational spectrum of Michler's ketone: experimental and theoretical investigations* Spectrochimica Acta A. 2014, Vol. 131, s. 678–685.
55. Staśkiewicz B., Turowska-Tyrk I., Baran J., Górecki C., Czapla Z.: *Structural characterization, thermal, vibrational properties and molecular motions in perovskite-type diaminopropanetetrachlorocadmate  $NH_3(CH_2)_3NH_3CdCl_4$  crystal*. Journal of Physics and Chemistry of Solids. 2014, Vol. 75, No. 12, s. 1305–1317.
56. Strasburger K., Naciążek P.: *Electric dipole hyperpolarizability of the beryllium atom in the gas phase and in spatial confinement*. Journal of Physics B. 2014, Vol. 47, No. 2, s. 1–6.
57. Strasburger K.: *High angular momentum states of lithium atom, studied with symmetry-projected explicitly correlated Gaussian lobe functions*. Journal of Chemical Physics. 2014, Vol. 141, No. 4, art. 044104, s. 1–5.

58. Sworakowski J., Bielecka U., Lutsyk P., Janus K.: *Effect of spatial inhomogeneity of charge carrier mobility on current-voltage characteristics in organic field-effect transistors*. Thin Solid Films. 2014, Vol. 571, No. 1, s. 56–61.
59. Szabla R., Góra R., Šponer J., Šponer J.E.: *Molecular mechanism of diamino-maleonitrile to diaminofumaronitrile photoisomerization: an intermediate step in the prebiotic formation of purine nucleobases*. Chemistry: a European Journal. 2014, Vol. 20, No. 9, s. 2515–2521.
60. Szabla R., Šponer J.E., Šponer J., Sobolewski A.L., Góra R.: *Solvent effects on the photochemistry of 4-aminoimidazole-5-carbonitrile, a prebiotically plausible precursor of purines*. Physical Chemistry Chemical Physics. 2014, Vol. 16, No. 33, s. 17617–17626.
61. Szefczyk B., Roszak R., Roszak S.: *Structure of the hexagonal NaYF<sub>4</sub> phase from first-principles molecular dynamics*. RSC Advances. 2014, Vol. 4, No. 43, s. 22526–22535.
62. Szefczyk B., Sokalski A.: *Physical nature of intermolecular interactions in [BMIM][PF<sub>6</sub>] ionic liquid*. Journal of Physical Chemistry B. 2014, Vol. 118, No. 8, s. 2147–2156.
63. Szeremeta J., Nyk M.W., Samoć M.: *Photocurrent enhancement in polythiophene doped with silver nanoparticles*. Optical Materials (Amsterdam). 2014, Vol. 37, s. 688–694.
64. Sznitko L., Cyprych K.M., Szukalski A., Miniewicz A., Myśliwiec J.: *Coherent-incoherent random lasing based on nano-rubbing induced cavities*. Laser Physics Letters. 2014, Vol. 11, No. 4, s. 1–5.
65. Szostak M.M., Pielak K.K., Hołderna-Natkaniec K., Natkaniec I., Bidzińska E.: *Optical nonlinearity and electric conductivity origin study on sucrose crystal by using IR, Raman, INS, NMR, and EPR spectroscopies*. Carbohydrate Research. 2014, Vol. 395, s. 29–37.
66. Szukalski A., Sznitko L., Cyprych K.M., Miniewicz A., Myśliwiec J.: *Light amplification in derivatives of pyrazoline-based systems*. Journal of Physical Chemistry C. 2014, Vol. 118, No. 15, s. 8102–8110.
67. Tresset G., Tatou M., Le Cœur C., Zeghal M., Bailleux V., Lecchi A., Brach K., Klekotko M., Porcar L.: *Weighing polyelectrolytes packaged in viruslike particles*. Physical Review Letters. 2014, Vol. 113, art. 128305, s. 1–5.
68. Trzebiatowska-Gusowska M., Pliński E., Baran J., Walczakowski M., Jarzab P., Nowak K., Fuglewicz B., Mikulics M., Pałka N., Szustakowski M.: *Terahertz and*

- Raman spectra of non-centrosymmetrical organic molecular crystals*. Optical Materials (Amsterdam). 2014, Vol. 37, s. 28–35.
69. Vivas M.G., Da Silva D., Malinge J., Boujtita M., Zaleśny R., Bartkowiak W., Agren H., Canuto S., De Boni L., Ishow E., Mendonca C.R.: *Molecular structure – optical property relationships for a series of non-centrosymmetric two-photon absorbing push-pull triarylamine molecules*. Scientific Reports. 2014, Vol. 4, art. 4447, s. 1–11.
70. Wawrzyńczyk D.M., Nyk M.W., Bednarkiewicz A., Stręk W., Samoć M.: *Morphology- and size-dependent spectroscopic properties of Eu<sup>3+</sup>-doped Gd<sub>2</sub>O<sub>3</sub> colloidal nanocrystals*. Journal of Nanoparticle Research. 2014, Vol. 16, art. 2690, s. 1–13.
71. Zaleśny R.: *Anharmonicity contributions to the vibrational first and second hyperpolarizability of para-disubstituted benzenes*. Chemical Physics Letters. 2014, Vol. 595/596, s. 109–112.

## 2013

1. Anczykowska A., Bartkiewicz S., Myśliwiec J.: *Laser coherence meter based on nanostructured liquid crystals*. International Journal of Optics. 2013, Vol. 2013, s. 1–3.
2. Azenha M., Szefczyk B., Loureiro D., Kathirvel P., Cordeiro M., Natália D.S., Fernando-Silva A.: *Computational and experimental study of the effect of PEG in the preparation of damascenone-imprinted xerogels*. Langmuir. 2013, Vol. 29, No. 6, s. 2024–2032.
3. Baranowska-Łączkowska A., Bartkowiak W., Góra R., Pawłowski F., Zaleśny R.: *On the performance of long-range-corrected density functional theory and reduced-size polarized LPol-n basis sets in computations of electric dipole (hyper)polarizabilities of  $\pi$ -conjugated molecules*. Journal of Computational Chemistry. 2013, Vol. 34, No. 10, s. 819–826.
4. Baranowska-Łączkowska A., Fernández B., Zaleśny R.: *New basis sets for the evaluation of interaction-induced electric properties in hydrogen-bonded complexes*. Journal of Computational Chemistry. 2013, Vol. 34, No. 4, s. 275–283.
5. Barillé R., Samoć A., Luther-Davies B., Samoć M., Nunzi J.-M.: *Self-reconstructing all-optical poling in polymer fibers*. Optics Letters. 2013, Vol. 38, No. 16, s. 2945–2948.
6. Bednarska J.D., Roztoczyńska A.K., Bartkowiak W., Zaleśny R.: *Comparative assessment of density functionals for excited-state dipole moments*. Chemical Physics Letters. 2013, Vol. 584, s. 58–62.

7. Beker W.L., Langner K.M., Dyguda-Kazimierowicz E.B., Feliks M., Sokalski A.: *Low-cost prediction of relative stabilities of hydrogen bonded complexes from atomic multipole moments for overly short intermolecular distances*. Journal of Computational Chemistry. 2013, Vol. 34, No. 21, s. 1797–1799.
8. Beker W.L., Szarek P., Komorowski L., Lipiński J.: *Reactivity patterns of imidazole, oxazole, and thiazole as reflected by the polarization justified Fukui functions*. Journal of Physical Chemistry A. 2013, Vol. 117, No. 7, s. 1596–1600.
9. Bernini C., Andruniów T., Olivucci M., Pogni R., Basosi R., Sinicropi A.: *Effects of the protein environment on the spectral properties of tryptophan radicals in Pseudomonas aeruginosa azurin*. Journal of the American Chemical Society. 2013, Vol. 135, No. 12, s. 4822–4833.
10. Bielecka U., Lutsyk P., Nyk M.W., Janus K., Samoć M., Bartkowiak W., Nešpůrek S.: *Hole transport in organic field-effect transistors with active poly(3-hexylthiophene) layer containing CdSe quantum dots*. Materials Science-Poland. 2013, Vol. 31, No. 2, s. 288–297.
11. Bulik I.W., Zaleśny R., Bartkowiak W., Luis J.M., Kirtman B., Scuseria G.E., Avramopoulos A., Reis H., Papadopoulos M.G.: *Performance of density functional theory in computing nonresonant vibrational (hyper)polarizabilities*. Journal of Computational Chemistry. 2013, Vol. 34, No. 20, s. 1775–1784.
12. Cato M.A., Majumdar D., Roszak S., Leszczynski J.: *Exploring relative thermodynamic stabilities of formic acid and formamide dimers – role of low-frequency hydrogen-bond vibrations*. Journal of Chemical Theory and Computation. 2013, Vol. 9, No. 2, s. 1016–1026.
13. Chudyk E., Dyguda-Kazimierowicz E.B., Langner K.M., Sokalski A., Lodola A., Mor M., Sirirak J., Mulholland A.J.: *Nonempirical energetic analysis of reactivity and covalent inhibition of fatty acid amide hydrolase*. Journal of Physical Chemistry B. 2013, Vol. 117, No. 22, s. 6656–6666.
14. Cichy B., Wawrzyńczyk D.M., Bednarkiewicz A., Samoć M., Stręk W.: *Third-order nonlinear optical response of CuInS<sub>2</sub> quantum dots-bright probes for near-infrared biodetection*. Applied Physics Letters. 2013, Vol. 102, No. 24, art. 243702, s. 1–5.
15. Coe B.J., Foxon S.P., Helliwell M., Rusanova D., Brunschwig B.S., Clays K., Depotter G., Nyk M.W., Samoć M., Wawrzyńczyk D.M., Garín J., Orduna J.: *Heptametallic, octupolar nonlinear optical chromophores with six ferrocenyl substituents*. Chemistry: a European Journal. 2013, Vol. 19, No. 21, s. 6613–6629.
16. Costa R.D., Aragón J., Ortí E., Pappenfus T.M., Mann K.R., Matczyszyn K., Samoć M., Zafra J.L., López N., Juan T., Casado J.: *Impact of the synergistic*

- collaboration of oligothiophene bridges and ruthenium complexes on the optical properties of dumbbell-shaped compounds*. Chemistry: A European Journal. 2013, Vol. 19, No. 4, s. 1476–1488.
17. Czajkowski M., Dradrach K., Bartkiewicz S., Galewski Z.: *Pattern of liquid crystalline droplets induced by two beam interference in azobenzene derivative*. Optical Materials (Amsterdam). 2013, Vol. 35, No. 12, s. 2449–2455.
  18. Czyżnikowska Ż., Góra R., Zaleśny R., Bartkowiak W., Baranowska-Łączkowska A., Leszczynski J.: *The effect of intermolecular interactions on the electric dipole polarizabilities of nucleic acid base complexes*. Chemical Physics Letters. 2013, Vol. 555, s. 230–234.
  19. Ditkowski B., Holmes N., Rydzak J., Donczew M., Bezulska M., Ginda K., Kędzierski P., Zakrzewska-Czerwińska J., Kelemen G.H., Jakimowicz D.: *Dynamic interplay of ParA with the polarity protein, Scy, coordinates the growth with chromosome segregation in Streptomyces coelicolor*. Open Biology. 2013, Vol. 3, s. 1–13.
  20. Fang Z., Webster R.D., Samoć M., Lai Y.-H.: *Tuning two-photon absorption cross-sections for triphenylamine derivatives*. RSC Advances. 2013, Vol. 3, No. 39, s. 17914–17917.
  21. Filipczak K., Karolczak J., Lipkowski P., Filarowski A., Ziółek M.: *Photochromic cycle of 2'-hydroxyacetophenone azine studied by absorption and emission spectroscopy in different solvents*. Journal of Chemical Physics. 2013, Vol. 139, No. 10, art. 104305, s. 1–11.
  22. Góra R., Błasiak B.: *On the origins of large interaction-induced first hyperpolarizabilities in hydrogen-bonded  $\pi$ -electronic complexes*. Journal of Physical Chemistry A. 2013, Vol. 117, No. 31, s. 6859–6866.
  23. Góra R., Maj M., Grabowski S.J.: *Resonance-assisted hydrogen bonds revisited: resonance stabilization vs. charge delocalization*. Physical Chemistry Chemical Physics. 2013, Vol. 15, No. 7, s. 2514–2522.
  24. Hańczyc P., Samoć M., Nordén B.: *Multiphoton absorption in amyloid protein fibres*. Nature Photonics. 2013, Vol. 7, No. 12, s. 969–972.
  25. Jaworska J., Bartkiewicz S., Galewski Z.: *Phase diagram of trans–cis isomers for photoactive and mesogenic 4-hexyl-4'-propoxyazobenzene*. Journal of Physical Chemistry C. 2013, Vol. 117, No. 51, s. 27067–27072.
  26. Jędrzejewska B., Krawczyk P., Pietrzak M., Gordel M., Matczyszyn K., Samoć M., Cysewski P.: *Styryl dye possessing donor- $\pi$ -acceptor structure – synthesis, spectroscopic and computational studies*. Dyes and Pigments. 2013, Vol. 99, No. 3, s. 673–685.

27. Jędrzejewski M., Ordon P., Komorowski L.: *Variation of the electronic dipole polarizability on the reaction path*. Journal of Molecular Modeling. 2013, Vol. 19, No. 10, s. 4203–4207.
28. Kozłowska J.J., Wielgus M.E., Bartkowiak W.: *TD-DFT study on the charge-transfer excitations of anions possessing double or triple bonds*. Computational and Theoretical Chemistry. 2013, Vol. 1014, s. 49–55.
29. Łączkowski K.Z., Czyżnikowska Ż., Zaleśny R., Baranowska-Łączkowska A.: *The B-H-B bridging interaction in B-substituted oxazaborolidine–borane complexes: a theoretical study*. Structural Chemistry. 2013, Vol. 24, No. 5, s. 1485–1492.
30. Maj M., Jeon J., Góra R., Cho M.: *Induced optical activity of DNA-templated cyanine dye aggregates: exciton coupling theory and TD-DFT studies*. Journal of Physical Chemistry A. 2013, Vol. 117, No. 29, s. 5909–5918.
31. Manea A., Rau I., Tane A., Kajzar F., Sznitko L., Miniewicz A.: *Poling kinetics and second order NLO properties of DCNP doped PMMA based thin film*. Optical Materials (Amsterdam). 2013, Vol. 36, No. 1, s. 69–74.
32. Massue J., Olesiak-Bańska J., Jeanneau E., Aronica C., Matczyszyn K., Samoć M., Monnereau C., Andraud C.: *Remarkable effect of iridium cyclometalation on the nonlinear absorption properties of a quadrupolar imine ligand*. Inorganic Chemistry. 2013, Vol. 52, No. 19, s. 10705–10707.
33. Misiaszek T., Knapik K., Gaĝor A., Trzebiatowska-Gusowska M.: *Non-isostructural arrangement in the crystals of 2-bromo- and 2-iodobenzyl alcohols: the influence of Br-Br interactions*. Journal of Molecular Structure. 2013, Vol. 1054/1055, s. 117–122.
34. Musiał T., Videnova-Adrabińska V., Turowska-Tyrk I., Duczmal M., Jerzykiewicz M.: *Synthesis, crystal structure and magnetic properties of a novel copper(II) complex with sulfoisophthalic acid*. Journal of Molecular Structure. 2013, Vol. 1054/1055, s. 134–142.
35. Olesiak-Bańska J., Gordel M., Matczyszyn K., Shynkar V., Zyss J., Samoć M.: *Gold nanorods as multifunctional probes in a liquid crystalline DNA matrix*. Nanoscale. 2013, Vol. 5, No. 22, s. 10975–10981.
36. Olesiak-Bańska J., Matczyszyn K., Zaleśny R., Murugan N.A., Kongsted J., Agren H., Bartkowiak W., Samoć M.: *Revealing spectral features in two-photon absorption spectrum of Hoechst 33342: a combined experimental and quantum-chemical study*. Journal of Physical Chemistry B. 2013, Vol. 117, No. 40, s. 12013–12019.

37. Piela K.K., Hołderna-Natkaniec K., Baranowski M., Misiaszek T., Baran J., Szostak M.M.: *Molecular motions contributions to optical nonlinearity of N-benzyl-2-methyl-4-nitroaniline studied by temperature-dependent FT-IR, 1H NMR spectroscopy and DFT calculations*. Journal of Molecular Structure. 2013, Vol. 1033, s. 91–97.
38. Roztoczyńska A.K., Kaczmarek-Kędziera A., Góra R., Bartkowiak W.: *How does the Boys and Bernardi counterpoise correction scheme affects the calculated interaction-induced electric properties? Model hydrogen-bonded systems as a case study*. Chemical Physics Letters. 2013, Vol. 571, s. 28–33.
39. Salomon A., Zielinski M., Kołkowski R., Zyss J., Prior Y.: *Size and shape resonances in second harmonic generation from silver nanocavities*. Journal of Physical Chemistry C. 2013, Vol. 117, No. 43, s. 22377–22382.
40. Sitkiewicz S.P., Mikołajczyk M., Toman P., Zaleśny R., Bartkowiak W.: *Towards first-principles based modeling of poly-3-alkylthiophenes: the nature of interactions in 2,2'-bithiophene dimer*. Chemical Physics Letters. 2013, Vol. 566, s. 67–70.
41. Sobolewska A.M., Bartkiewicz S., Myśliwiec J.: *Reversible optical memory based on single-component phototropic liquid crystal*. Applied Physics Letters. 2013, Vol. 103, No. 8, art. 083302, s. 1–4.
42. Sobolewska A.M., Noga J.E., Bartkiewicz S., Galewski Z.: *Mechanism of photochemical phase transition of single-component phototropic liquid crystals studied by means of holographic grating recording*. Journal of Physical Chemistry C. 2013, Vol. 117, No. 19, s. 10051–10058.
43. Szabla R., Šponer J.E., Šponer J., Góra R.: *Theoretical studies of the mechanism of 2-aminooxazole formation under prebiotically plausible conditions*. Physical Chemistry Chemical Physics. 2013, Vol. 15, No. 20, s. 7812–7818.
44. Szabla R., Tuna D., Góra R., Šponer J., Sobolewski A.L., Domcke W.: *Photochemistry of 2-aminooxazole, a hypothetical prebiotic precursor of RNA nucleotides*. Journal of Physical Chemistry Letters. 2013, Vol. 4, No. 16, s. 2785–2788.
45. Szeremeta J., Kołkowski R., Nyk M.W., Samoć M.: *Wavelength dependence of the complex third-order nonlinear optical susceptibility of poly(3-hexylthiophene) studied by femtosecond Z-scan in solution and thin film*. Journal of Physical Chemistry C. 2013, Vol. 117, No. 49, s. 26197–26203.
46. Szeremeta J., Nyk M.W., Wawrzyńczyk D.M., Samoć M.: *Wavelength dependence of nonlinear optical properties of colloidal CdS quantum dots*. Nanoscale. 2013, Vol. 5, No. 6, s. 2388–2393.

47. Sznitko L., Karpiński P., Bartkiewicz S., Miniewicz A., Myśliwiec J.: *Surface relief grating formation in luminescent dye doped photochromic polymer containing azobenzene side groups*. Central European Journal of Physics. 2013, Vol. 11, No. 8, s. 1024–1029.
48. Sznitko L., Parafiniuk K., Miniewicz A., Rau I., Kajzar F., Nizioł J., Hebda E., Pielichowski J., Sahraoui B., Myśliwiec J.: *Influence of surfactant on dynamics of photoinduced motions and light emission of a dye-doped deoxyribonucleic acid*. Optical Materials (Amsterdam). 2013, Vol. 35, No. 12, s. 2389–2393.
49. Sznitko L., Szukalski A., Cyprych K.M., Karpiński P., Miniewicz A., Myśliwiec J.: *Surface roughness induced random lasing in bio-polymeric dye doped film*. Chemical Physics Letters. 2013, Vol. 576, s. 31–34.
50. Szostak M.M., Chojnacki H., Piela K.K., Bidzińska E., Dyrek K.: *Oscillatory polarons generation by near IR and spin induced chirality studies in optically nonlinear 1,3-dinitrobenzene crystal*. Optical Materials (Amsterdam). 2013, Vol. 35, No. 5, s. 1004–1012.
51. Tane A., Kajzar F., Zgarian R., Rau I., Grabarek D., Karpiński P., Miniewicz A.: *Refractive index and surface relief grating formation in DNA based dye-doped films*. Macromolecular Research. 2013, Vol. 21, No. 3, s. 331–337.
52. Tarasiewicz J., Jakubas R., Majerz I., Baran J., Gaḡor A., Miniewicz A.: *The IR temperature studies of phase transition of 4-aminopyridinium-hydrogen maleate-maleic acid: isotopic effect and nonlinear optical properties*. Vibrational Spectroscopy. 2013, Vol. 66, s. 93–103.
53. Toczek D., Kubas K., Turek M., Roszak S., Gancarz R.: *Theoretical studies of structure, energetics and properties of  $Ca^{2+}$  complexes with alizarin glucoside*. Journal of Molecular Modeling. 2013, Vol. 19, No. 10, s. 4209–4214.
54. Tomczyk J., Sobolewska A.M., Nagy Z.T., Guillon D., Donnio B., Stumpe J.: *Photo- and thermal-processing of azobenzene-containing star-shaped liquid crystals*. Journal of Materials Chemistry. C. 2013, Vol. 1, No. 5, s. 924–932.
55. Vivas M.G., Da Silva D., De Boni L., Bretonniere Y., Andraud C., Laibe-Darbour F., Mulatier J.C., Zaleśny R., Bartkowiak W., Canuto S., Mendonca C.R.: *Revealing the electronic and molecular structure of randomly oriented molecules by polarized two-photon spectroscopy*. Journal of Physical Chemistry Letters. 2013, Vol. 4, No. 10, s. 1753–1759.
56. Walczak E.B., Szcfczyk B., Andruniów T.: *Geometries and vertical excitation energies in retinal analogues resolved at the CASPT2 level of theory: critical assessment of the performance of CASSCF, CC2, and DFT methods*. Journal of Chemical Theory and Computation. 2013, Vol. 9, No. 11, s. 4915–4927.

57. Wawrzyńczyk D.M., Bednarkiewicz A., Nyk M.W., Stręk W., Samoć M.: *Ligand-dependent luminescence of ultra-small Eu<sup>3+</sup>-doped NaYF<sub>4</sub> nanoparticles*. Journal of Nanoparticle Research. 2013, Vol. 15, No. 6, art. 1707, s. 1–11.
58. Wawrzyńczyk D.M., Nyk M.W., Bednarkiewicz A., Stręk W., Samoć M.: *A comparison of morphology, structure and optical properties of ultrasmall, small and core-shell up-converting NaYF<sub>4</sub>/NaGdF<sub>4</sub> nanocrystals co-doped with Tm<sup>3+</sup> and Yb<sup>3+</sup> ions*. Journal of Luminescence. 2013, Vol. 133, s. 138–144.
59. Wawrzyńczyk D.M., Nyk M.W., Samoć M.: *Multiphoton absorption in europium(III) doped YVO<sub>4</sub> nanoparticles*. Journal of Materials Chemistry. C. 2013, Vol. 1, No. 37, s. 5837–5842.
60. Wielgus M.E., Zaleśny R., Murugan N.A., Kongsted J., Agren H., Samoć M., Bartkowiak W.: *Two-photon solvatochromism. 2, Experimental and theoretical study of solvent effects on the two-photon absorption spectrum of reichardt's dye*. ChemPhysChem. 2013, Vol. 14, No. 16, s. 3731–3739.
61. Wojaczyńska E., Turowska-Tyrk I.: *Autoxidation of a tetracyclic lactam and its conversion to an enantiopure tertiary alcohol*. Tetrahedron: Asymmetry. 2013, Vol. 24, No. 19, s. 1247–1251.
62. Wołczyr M., Strasburger K., Chojnacki H.: *Two-photon annihilation rate of the positronic HCN molecule*. Molecular Physics. 2013, Vol. 111, No. 2, s. 345–352.
63. Zakrzewska A., Zaleśny R., Kolehmainen E., Ośmiałowski B., Jędrzejewska B., Agren H., Pietrzak M.: *Substituent effects on the photophysical properties of fluorescent 2-benzoylmethylenequinoline difluoroboranes: a combined experimental and quantum chemical study*. Dyes and Pigments. 2013, Vol. 99, No. 3, s. 957–965.
64. Zaleśny R., Góra R., Kozłowska J.J., Luis J.M., Agren H., Bartkowiak W.: *Resonant and nonresonant hyperpolarizabilities of spatially confined molecules: a case study of cyanoacetylene*. Journal of Chemical Theory and Computation. 2013, Vol. 9, No. 8, s. 3463–3472.
65. Zierkiewicz W., Zaleśny R., Hobza P.: *On the nature of unusual intensity changes in the infrared spectra of the enflurane-acetone complexes*. Physical Chemistry Chemical Physics. 2013, Vol. 15, No. 16, s. 6001–6007.

## 2012

1. Anczykowska A., Bartkiewicz S., Nyk M.W., Myśliwiec J.: *Study of semiconductor quantum dots influence on photorefractivity of liquid crystals*. Applied Physics Letters. 2012, Vol. 101, No. 10, s. 101107(1–4).

2. Bąkowiec J.B., Siedlecka R., Turowska-Tyrk I.: *Monitoring structural transformations in crystals. Pt. 15, Structural changes in crystals caused by UV radiation despite the lack of a photochemical reaction.* Journal of Chemical Crystallography. 2012, Vol. 42, No. 6, s. 593–599.
3. Bąkowiec J.B., Turowska-Tyrk I.: *Photo-induced structural transformations in crystals at high pressure. Pt. 1, The crystallographic studies of the photochemical reaction at high pressure.* Journal of Photochemistry and Photobiology. A. 2012, Vol. 232, s. 41–43.
4. Barlow A., Babgi B., Samoć M., Corkery C.T., Cleuvenbergen S., Asselberghs I., Clays K., Cifuentes M.P., Humphrey M.G.: *Organometallic complexes for non-linear optics. [Pt.] 51, Second- and third-order non-linear optical properties of alkynylgold complexes.* Australian Journal of Chemistry. 2012, Vol. 65, No. 7, s. 834–841.
5. Bednarkiewicz A., Wawrzyńczyk D.M., Gagor A., Kępiński L., Kurnatowska M., Krajczyk L., Nyk M.W., Samoć M., Stręk W.: *Giant enhancement of upconversion in ultra-small  $Er^{3+}/Yb^{3+}:NaYF_4$  nanoparticles via laser annealing.* Nanotechnology. 2012, Vol. 23, No. 14, s. 1–8.
6. Boratyński P., Turowska-Tyrk I., Skarżewski J.: *Synthetic approaches to 9-arylated Cinchona alkaloids: stereoselective addition of Grignard reagents to cinchonones and hydroxylation of 9-phenylcinchonanes.* Tetrahedron: Asymmetry. 2012, Vol. 23, No. 11/12, s. 876–883.
7. Cabaj J., Chyla A., Jędrychowska A.U., Olech K., Sołducho J.: *Detecting platform for phenolic compounds – characteristic of enzymatic electrode.* Optical Materials (Amsterdam). 2012, Vol. 34, No. 10, s. 1677–1681.
8. Cailleau H., Luty T., Koshihara S.Y., Servol M., Lorenc M., Buron-Le Cointe M., Collet E.: *PIPT from the beginning to future.* Acta Physica Polonica A. 2012, Vol. 121, No. 2, s. 297–306.
9. Ciosłowski J., Strasburger K., Matito E.: *The three-electron harmonium atom: the lowest-energy doublet and quadruplet states.* Journal of Chemical Physics. 2012, Vol. 136, No. 19, s. 194112(1–8).
10. Czajkowski M., Bartkiewicz S., Myśliwiec J.: *Growth of isotropic domains as a mechanism of dynamic diffraction grating recording in low molecular liquid-crystalline derivatives of azobenzene.* Journal of Physical Chemistry B. 2012, Vol. 116, No. 10, s. 3264–3269.
11. Czajkowski M., Bartkiewicz S., Myśliwiec J.: *Light-stimulated growth of isotropic domains in nematic liquid crystal.* Chemical Physics Letters. 2012, Vol. 550, s. 73–78.

12. Drouet S., Merhi A., Grelaud G., Cifuentes M.P., Humphrey M.G., Matczyszyn K., Samoć M., Toupet L., Paul-Roth C.O., Paul F.: *Enhanced two-photon absorption cross-sections of zinc(II) tetraphenylporphyrins peripherally substituted with d6-metal alkynyl complexes*. New Journal of Chemistry. 2012, Vol. 36, No. 11, s. 2192–2195.
13. Drouet S., Merhi A., Yao D., Cifuentes M.P., Humphrey M.G., Wielgus M.E., Olesiak-Bańska J., Matczyszyn K., Samoć M., Paul F., Paul-Roth C.O.: *Cubic nonlinear optical properties of new zinc tetraphenyl porphyrins peripherally functionalized with electron-rich Ru(II) alkynyl substituents*. Tetrahedron. 2012, Vol. 68, No. 50, s. 10351–10359.
14. Gatri R., Fillaut J.-L., Myśliwiec J., Szukalski A., Bartkiewicz S., El-Ouazzani H., Guezguez I., Khammar F., Sahraoui B.: *Synthesis and characterization of azo-containing organometallic thin films for all optical switching applications*. Chemical Physics Letters. 2012, Vol. 535, s. 106–110.
15. Góra R., Zaleśny R., Kozłowska J.J., Naciążek P., Roztoczyńska A.K., Strasburger K., Bartkowiak W.: *Electric dipole (hyper)polarizabilities of spatially confined LiH molecule*. Journal of Chemical Physics. 2012, Vol. 137, No. 9, s. 094307(1–10).
16. Green K.A., Simpson P.V., Corkery C.T., Cifuentes M.P., Samoć M., Humphrey M.G.: *Divergent synthesis of ruthenium alkynyl dendrimers and a two-photon absorption cross-section dendritic effect*. Macromolecular Rapid Communications. 2012, Vol. 33, No. 6/7, s. 573–578.
17. Gusowski A.M., Swart H.C., Karlsson L.S., Trzebiatowska-Gusowska M.: *NaYF<sub>4</sub>:Pr<sup>3+</sup> nanocrystals displaying photon cascade emission*. Nanoscale. 2012, Vol. 4, No. 2, s. 541–546.
18. Hańczyc P., Åkerman B., Nordén B.: *Short oligonucleotides aligned in stretched humid matrix: secondary DNA structure in poly(vinyl alcohol) environment*. Langmuir. 2012, Vol. 28, No. 16, s. 6662–6669.
19. Hańczyc P., Nordén B., Samoć M.: *Two-photon absorption of metal – organic DNA-probes*. Dalton Transactions. 2012, Vol. 41, No. 11, s. 3123–3125.
20. Jabłoński M., Sokalski A.: *Physical nature of interactions in charge-inverted hydrogen bonds*. Chemical Physics Letters. 2012, Vol. 552, s. 156–161.
21. Karpieński P., Miniewicz A.: *Optical phase conjugation in azo-dye doped chiral liquid crystal*. Applied Physics Letters. 2012, Vol. 101, No. 16, s. 161108(1–4).

22. Langner K.M., Beker W.L., Sokalski A.: *Robust predictive power of the electrostatic term at shortened intermolecular distances*. Journal of Physical Chemistry Letters. 2012, Vol. 3, s. 2785–2789.
23. Łapkowski M., Data P., Nowakowska-Oleksy A., Sołoducho J., Roszak S.: *Electrochemical characterization of alternate conducting carbazole-bisthiophene units*. Materials Chemistry and Physics. 2012, Vol. 131, No. 3, s. 757–763.
24. Lutsyk P., Janus K., Sworakowski J., Kochalska A., Nešpůrek S.: *Kinetic study of light-driven processes in photochromic dye-doped polymers used as gate insulators in photoswitchable organic field effect transistors*. Chemical Physics. 2012, Vol. 404, s. 22–27.
25. Majumdar D., Roszak S., Leszczynski J.: *Theoretical studies on the structure and electronic properties of cubic gold nanoclusters*. Canadian Journal of Chemical Engineering. 2012, Vol. 90, No. 4, s. 852–859.
26. Martyniak A., Lipkowski P., Boens N., Filarowski A.: *Electron-topological, energetic and  $\pi$ -electron delocalization analysis of ketoenamine-enolimine tautomeric equilibrium*. Journal of Molecular Modeling. 2012, Vol. 18, No. 1, s. 257–263.
27. Matczyszyn K., Olesiak-Bańska J.: *DNA as scaffolding for nanophotonic structures*. Journal of Nanophotonics. 2012, Vol. 6, No. 1, art. 064505, s. 1–15.
28. Mazur L.M., Kolkowski R., Matczyszyn K., Mathevet F., Rannou P., Attias A.-J., Samoć M.: *Spectral dependence of nonlinear absorption and refraction in terthiophene-based organic semiconductors*. Optical Materials (Amsterdam). 2012, Vol. 34, No. 10, s. 1682–1685.
29. Mikołajczyk M., Czyżnikowska Ż., Czeleń P., Bielecka U., Zaleśny R., Toman P., Bartkowiak W.: *Quantum chemical study of hole transfer coupling in nucleic acid base complexes containing 7-deazaadenine*. Chemical Physics Letters. 2012, Vol. 537, s. 94–100.
30. Myśliwiec J., Czajkowski M., Bartkiewicz S., Żygadło K., Galewski Z., Sahraoui B.: *Applications of low molecular liquid crystalline derivatives of azobenzene*. Non-linear Optics, Quantum Optics. 2012, Vol. 45, No. 1/2, s. 93–100.
31. Myśliwiec J., Sznitko L., Szukalski A., Parafiniuk K., Bartkiewicz S., Miniewicz A., Sahraoui B., Rau I., Kajzar F.: *Amplified spontaneous emission of 3-(1,1-dicyanoethenyl)-1-phenyl-4,5-dihydro-1H-pyrazole molecule embedded in various polymer matrices*. Optical Materials (Amsterdam). 2012, Vol. 34, No. 10, s. 1725–1728.
32. Nyk M.W., Wawrzyńczyk D.M., Szeremeta J., Samoć M.: *Spectrally resolved size-dependent third-order nonlinear optical properties of colloidal CdSe quantum dots*. Applied Physics Letters. 2012, Vol. 100, No. 4, s. 041102(1–4).

33. Olesiak-Bańska J., Gordel M., Kołkowski R., Matczyszyn K., Samoć M.: *Third-order nonlinear optical properties of colloidal gold nanorods*. Journal of Physical Chemistry C. 2012, Vol. 116, No. 25, s. 13731–13737.
34. Olesiak-Bańska J., Hańczyc P., Matczyszyn K., Nordén B., Samoć M.: *Nonlinear absorption spectra of ethidium and ethidium homodimer*. Chemical Physics. 2012, Vol. 404, s. 33–35.
35. Olsztyńska-Janus S., Gąsior-Głogowska M.E., Szymborska-Małek K., Komorowska M., Witkiewicz W., Pezowicz C., Szotek S., Kobielarz J.: *Spectroscopic techniques in the study of human tissues and their components. Pt. 2, Raman spectroscopy*. Acta of Bioengineering and Biomechanics. 2012, Vol. 14, No. 4, s. 121–133.
36. Olsztyńska-Janus S., Szymborska-Małek K., Gąsior-Głogowska M.E., Walski T.J., Komorowska M., Witkiewicz W., Pezowicz C., Kobielarz M.J., Szotek S.: *Spectroscopic techniques in the study of human tissues and their components. Pt. 1, IR spectroscopy*. Acta of Bioengineering and Biomechanics. 2012, Vol. 14, No. 3, s. 101–115.
37. Owczarek M., Szklarz P., Jakubas R., Miniewicz A.: *[NH<sub>2</sub>(C<sub>2</sub>H<sub>4</sub>)<sub>2</sub>O]MX<sub>5</sub>: A new family of morpholinium nonlinear optical materials among halogenoantimonate(III) and halogenobismuthate(III) compounds: structural characterization, dielectric and piezoelectric properties*. Dalton Transactions. 2012, Vol. 41, No. 24, s. 7285–7294.
38. Palewska K., Sworakowski J., Lipiński J.: *Molecular aggregation in soluble phthalocyanines – chemical interactions vs.  $\pi$ -stacking*. Optical Materials (Amsterdam). 2012, Vol. 34, No. 10, s. 1717–1724.
39. Pawlik G., Mituś A., Karpiński P., Miniewicz A.: *Laser light-induced molecular reorientation in 90° twisted nematic liquid crystal: classic approach, Monte Carlo modeling and experiment*. Optical Materials (Amsterdam). 2012, Vol. 34, No. 10, s. 1697–1703.
40. Pawlik G., Mituś A., Miniewicz A.: *Modelling of enhanced photoinduced reorientation of nematic liquid crystal molecules in twisted geometry: Monte Carlo approach*. Molecular Crystals and Liquid Crystals. 2012, Vol. 554, No. 1, s. 56–64.
41. Piela K.K., Kozankiewicz B., Lipiński J., Szostak M.M.: *Low temperature emission spectra of optically nonlinear N-benzyl-2-methyl-4-nitroaniline crystal*. Chemical Physics. 2012, Vol. 404, s. 28–32.
42. Piela K.K., Szostak M.M.: *Electrical anharmonicity and vibronic couplings contributions to optical nonlinearity of N-benzyl-2-methyl-4-nitroaniline crystal studied by FT-IR, polarized FT-NIR, resonance Raman and UV-Vis spectroscopy*. Journal of Physical Chemistry A. 2012, Vol. 116, No. 7, s. 1730–1745.

43. Radościński Ł., Luty T., Nasu K., Ohnishi H., Nishioka K., Radosz A., Wójt D.: *Photoinduced conversion of hybridization in graphite*. Acta Physica Polonica A. 2012, Vol. 121, No. 2, s. 359–368.
44. Rau I., Szukalski A., Sznitko L., Miniewicz A., Bartkiewicz S., Kajzar F., Sahraoui B., Myśliwiec J.: *Amplified spontaneous emission of Rhodamine 6G embedded in pure deoxyribonucleic acid*. Applied Physics Letters. 2012, Vol. 101, No. 17, s. 171113(1–3).
45. Roszak R., Góra R., Roszak S.: *The theoretical studies of interactions of the  $\text{OH}^-(\text{H}_2\text{O})_n$  clusters evolution toward the hydroxide anion hydration*. International Journal of Quantum Chemistry. 2012, Vol. 112, No. 18, s. 3046–3051.
46. Roztoczyńska A.K., Góra R., Mikołajczyk M., Bartkowiak W.: *On the calculations of interaction energies and induced electric properties within the polarizable continuum model*. Journal of Physical Chemistry A. 2012, Vol. 116, No. 17, s. 4409–4416.
47. Roztoczyńska A.K., Kaczmarek-Kędziera A., Bartkowiak W.: *On the potential application of DFT methods in predicting the interaction-induced electric properties of molecular complexes: molecular H-bonded chains as a case of study*. Journal of Molecular Modeling. 2012, Vol. 18, No. 7, s. 3073–3086.
48. Ryabchun A., Bobrovsky A., Sobolewska A.M., Shibaev V., Stumpe J.: *Dual photorecording on cholesteric azobenzene-containing LC polymer films using helix pitch phototuning and holographic grating recording*. Journal of Materials Chemistry. 2012, Vol. 22, No. 13, s. 6245–6250.
49. Saint-Jalm S., Miniewicz A., Karpiński P., Jarek M.U., Galewski Z.: *Photo-induced birefringence in a nematic liquid crystal mixture doped with light-switchable mesogenic azobenzene derivatives*. Journal of Molecular Liquids. 2012, Vol. 168, s. 21–27.
50. Schab-Balcerzak E., Sobolewska A.M., Stumpe J., Hamryszak Ł., Bujak P.: *Surface relief gratings in azobenzene supramolecular systems based on polyimides*. Optical Materials (Amsterdam). 2012, Vol. 35, No. 2, s. 155–167.
51. Sobolewska A.M., Bartkiewicz S.: *Origin of the oscillations in the self-diffracted signal in degenerate-two wave mixing experiment in azo-polymer*. Applied Physics Letters. 2012, Vol. 100, No. 23, s. 233301(1–4).
52. Sobolewska A.M., Bartkiewicz S.: *Surface relief grating in azo-polymer obtained for s-s polarization configuration of the writing beams*. Applied Physics Letters. 2012, Vol. 101, No. 19, s. 193301(1–4).

53. Vivas M.G., Da Silva D., De Boni L., Bretonniere Y., Andraud C., Laibe-Darbour F., Mulatier J.C., Zalesny R., Bartkowiak W., Canuto S., Mendonca C.R.: *Experimental and theoretical study on the one- and two-photon absorption properties of novel organic molecules based on phenylacetylene and azoaromatic moieties*. Journal of Physical Chemistry B. 2012, Vol. 116, No. 50, s. 14677–14688.
54. Wawrzyńczyk D.M., Bednarkiewicz A., Nyk M.W., Cichos J., Karbowski M., Hreniak D., Stręk W., Samoć M.: *Optimisation of ligand exchange towards stable water suspensions of crystalline NaYF<sub>4</sub>: Er<sup>3+</sup>, Yb<sup>3+</sup> nanoluminophors*. Journal of Nanoscience and Nanotechnology. 2012, Vol. 12, No. 3, s. 1886–1891.
55. Wawrzyńczyk D.M., Bednarkiewicz A., Nyk M.W., Gordel M., Stręk W., Samoć M.: *Modulation of up-conversion luminescence of lanthanide(III) ion co-doped NaYF<sub>4</sub> nanoparticles using gold nanorods*. Optical Materials (Amsterdam). 2012, Vol. 34, No. 10, s. 1708–1712.
56. Wawrzyńczyk D.M., Bednarkiewicz A., Nyk M.W., Stręk W., Samoć M.: *Neodymium(III) doped fluoride nanoparticles as non-contact optical temperature sensors*. Nanoscale. 2012, Vol. 4, No. 22, s. 6959–6961.
57. Wielgus M.E., Bartkowiak W., Samoć M.: *Two-photon solvatochromism. I, Solvent effects on two-photon absorption cross section of 4-dimethylamino-4'-nitrostilbene (DANS)*. Chemical Physics Letters. 2012, Vol. 554, s. 113–116.
58. Wierzbicka C., Nyk M.W., Skowerski K., Samoć M.: *Molecules of ruthenium-based olefin metathesis catalysts as two- and three-photon absorbers*. 2012, Vol. 41, No. 43, s. 13258–13260.
59. Wojaczyńska E., Turowska-Tyrk I., Skarżewski J.: *Novel chiral bridged azepanes: stereoselective ring expansion of 2-azanorbornan-3-yl methanols*. Tetrahedron. 2012, Vol. 68, No. 38, s. 7848–7854.
60. Wołczyr M., Strasburger K.: *Modified adiabatic method: bound state of the e+HF molecule*. Journal of Physics B. 2012, Vol. 45, No. 8, s. 1–7.
61. Zegadlo K.B., Ouazzani H.E., Cieslik I., Weglowski R., Zmija J., Klosowicz S., Majchrowski A., Myśliwiec J., Sahraoui B., Karpierz M.A.: *Nonlinear optical properties of polymer dispersed liquid crystals doped with La<sub>2</sub>CaB<sub>10</sub>O<sub>19</sub>*. Optical Materials (Amsterdam). 2012, Vol. 34, No. 10, s. 1704–1707.

## 2011

1. Anczykowska A., Bartkiewicz S., Nyk M.W., Myśliwiec J.: *Enhanced photorefractive effect in liquid crystal structures co-doped with semiconductor quantum*

- dots and metallic nanoparticles*. Applied Physics Letters. 2011, Vol. 99, No. 19, s. 191109(1–3).
- Azenha M., Szeferczyk B., Loureiro D., Kathirvel P., Cordeiro M.N.D.S., Fernando-Silva A.: *Molecular dynamics simulations of pregelification mixtures for the production of imprinted xerogels*. Langmuir. 2011, Vol. 27, No. 8, s. 5062–5070.
  - Ba Tai T., Kadłubański P., Roszak S., Majumdar D., Leszczynski J., Nguyen M.T.: *Electronic structures and thermochemical properties of the small silicon-doped boron clusters  $B_nSi$  ( $n=1-7$ ) and their anions*. ChemPhysChem. 2011, Vol. 12, No. 16, s. 2948–2958.
  - Bąkiewicz J.B., Skarzewski J., Turowska-Tyrk I.: *Monitoring structural transformations in crystals. Pt. 14, Photo-induced structural changes in two crystal forms with different numbers of independent molecules*. CrystEngComm. 2011, Vol. 13, s. 4332–4338.
  - Bednarkiewicz A., Wawrzyńczyk D.M., Nyk M.W., Samoć M.: *Tuning red-green-white up-conversion color in nano  $NaYF_4:Er/Yb$  phosphor*. Journal of Rare Earths. 2011, Vol. 29, No. 12, s. 1152–1156.
  - Bednarkiewicz A., Wawrzyńczyk D.M., Nyk M.W., Stręk W.: *Optically stimulated heating using  $Nd^{3+}$  doped  $NaYF_4$  colloidal near infrared nanophosphors*. Applied Physics B-Lasers and Optics. 2011, Vol. 103, No. 4, s. 847–852.
  - Bednarkiewicz A., Wawrzyńczyk D.M., Nyk M.W., Stręk W.: *Synthesis and spectral properties of colloidal  $Nd^{3+}$  doped  $NaYF_4$  nanocrystals*. Optical Materials (Amsterdam). 2011, Vol. 33, No. 10, s. 1481–1486.
  - Benková Z., Szeferczyk B., Cordeiro M.N.D.: *Molecular dynamics study of hydrated poly(ethylene oxide) chains grafted on siloxane surface*. Macromolecules. 2011, Vol. 44, No. 9, s. 3639–3648.
  - Bielecka U., Lutsyk P., Janus K., Sworakowski J., Bartkowiak W.: *Effect of solution aging on morphology and electrical characteristics of regioregular P3HT FETs fabricated by spin coating and spray coating*. Organic Electronics. 2011, Vol. 12, No. 11, s. 1768–1776.
  - Cabaj J., Sołoducho J., Chyla A., Jędrychowska A.U.: *Hybrid phenol biosensor based on modified phenoloxidase electrode*. Sensors and Actuators. B, Chemical. 2011, Vol. 157, No. 1, s. 225–231.
  - Czajkowski M., Myśliwiec J., Żygadło K., Galewski Z., Bartkiewicz S.: *Temperature influence on dynamics of diffraction grating formation in systems based on photochromic liquid crystalline molecules*. Chemical Physics Letters. 2011, Vol. 510, No. 1–3, s. 131–134.

12. Czyżnikowska Ż., Bartkowiak W.: *Physical origins of the stability of aromatic amino acid core ring-polycyclic hydrocarbon complexes: a post-Hartree-Fock and density functional study*. Journal of Computational Chemistry. 2011, Vol. 32, No. 9, s. 1887–1895.
13. Gągor A., Piecha A., Jakubas R., Miniewicz A.: *Crystal structure and characterization of a novel acentric imidazolium analog  $[C_3N_2H_5^+][Br^-]$* . Chemical Physics Letters. 2011, Vol. 503, No. 1–3, s. 134–138.
14. Gauthier N., Argouarch G., Paul F., Toupet L., Ladjarafi A., Costuas K., Halet J.-F., Samoć M., Cifuentes M.P., Corkery C.T., Humphrey M.G.: *Electron-rich iron/ruthenium arylalkynyl complexes for third-order nonlinear optics: redox-switching between three states*. Chemistry: a European Journal. 2011, Vol. 17, No. 20, s. 5561–5577.
15. Góra R., Zaleśny R., Roztoczyńska A.K., Bartkowiak W., Skwara B., Papadopoulos M.G., Da Silva D.: *Large changes of static electric properties induced by hydrogen bonding: an ab initio study of linear HCN oligomers*. Journal of Physical Chemistry A. 2011, Vol. 115, No. 18, s. 4691–4700.
16. Grabowski S.J., Lipkowski P.: *Characteristics of X-H- $\pi$  interactions: ab initio and QTAIM studies*. Journal of Physical Chemistry A. 2011, Vol. 115, No. 18, s. 4765–4773.
17. Green K.A., Cifuentes M.P., Samoć M., Humphrey M.G.: *Metal alkynyl complexes as switchable NLO systems*. Coordination Chemistry Reviews. 2011, Vol. 255, No. 21/22, s. 2530–2541.
18. Green K.A., Cifuentes M.P., Samoć M., Humphrey M.G.: *Syntheses and NLO properties of metal alkynyl dendrimers*. Coordination Chemistry Reviews. 2011, Vol. 255, No. 17/18, s. 2025–2038.
19. Hańczyc P., Matczyszyn K., Pawlik K., Olesiak-Bańska J., Leh H., Buckle M.: *Spontaneous formation of liquid crystalline phases and phase transitions in highly concentrated plasmid DNA*. Liquid Crystals. 2011, Vol. 38, No. 4, s. 461–468.
20. Hańczyc P., Nordén B., Åkerman B.: *DNA in a polyvinyl alcohol matrix and interactions with three intercalating cyanine dyes*. Journal of Physical Chemistry B. 2011, Vol. 115, No. 42, s. 12192–12201.
21. He Guang S., Zhu J., Baev A., Samoć M., Frattarelli D.L., Watanabe N., Facchetti A., Agren H., Marks T.J., Prasad P.N.: *Twisted  $\pi$ -system chromophores for all-optical switching*. Journal of the American Chemical Society. 2011, Vol. 133, No. 17, s. 6675–6680.
22. Henry D.J., Szarek P., Hirai K., Ichikawa K., Tachibana A., Yarovsky I.: *Reactivity and regioselectivity of aluminum nanoclusters: insights from regional density*

- functional theory*. Journal of Physical Chemistry C. 2011, Vol. 115, No. 5, s. 1714–1723.
23. Ichikawa K., Ikeda Y., Wagatsuma A., Watanabe K., Szarek P., Tachibana A.: *Theoretical study of hydrogenated tetrahedral aluminum clusters*. International Journal of Quantum Chemistry. 2011, Vol. 111, No. 14, s. 3548–3555.
  24. Ichikawa K., Wagatsuma A., Szarek P., Zhou C., Cheng H., Tachibana A.: *Electronic stress tensor analysis of hydrogenated palladium clusters*. Theoretical Chemistry Accounts. 2011, Vol. 130, No. 2/3, s. 531–542.
  25. Jaszuński M., Łach G., Strasburger K.: *NMR shielding constants in hydrogen molecule isotopomers*. Theoretical Chemistry Accounts. 2011, Vol. 129, No. 3/5, s. 325–330.
  26. Karpicz R., Gulbinas V., Lewanowicz A., Macernis M., Sulskus J., Valkunas L.: *Relaxation pathways of excited N-(triphenylmethyl)salicylideneimine in solutions*. Journal of Physical Chemistry A. 2011, Vol. 115, No. 10, s. 1861–1868.
  27. Karpiński P., Miniewicz A.: *Surface plasmon polariton excitation in metallic layer via surface relief gratings in photoactive polymer studied by the finite-difference time-domain method*. Plasmonics. 2011, Vol. 6, No. 3, s. 541–546.
  28. Komorowski L., Lipiński J., Szarek P., Ordon P.: *Polarization justified Fukui functions: the theory and applications for molecules*. Journal of Chemical Physics. 2011, Vol. 135, No. 1, s. 014109(1–8).
  29. Kornobis K., Kumar N., Wong B.M., Lodowski P., Jaworska M., Andruniów T., Ruud K., Kozłowski P.M.: *Electronically excited states of vitamin B12: benchmark calculations including time-dependent density functional theory and correlated ab initio methods*. Journal of Physical Chemistry A. 2011, Vol. 115, No. 7, s. 1280–1292.
  30. Król-Gracz A., Michalak E., Nowak P.M., Dyonizy A.: *Photo-induced chemical reduction of silver bromide to silver nanoparticles*. Central European Journal of Chemistry. 2011, Vol. 9, No. 6, s. 982–989.
  31. Król-Gracz A., Michalak E., Nowak P.M., Dyonizy A.: *Preparation and characterization of ultra-fine silver bromide suspension*. Challenges of Modern Technology. 2011, Vol. 2, No. 2, s. 38–42.
  32. Kuduk-Jaworska J., Chojnacki H., Jański J.J.: *Non-empirical quantum chemical studies on electron transfer reactions in trans- and cis-diamminedichloroplatinum(II) complexes*. Journal of Molecular Modeling. 2011, Vol. 17, No. 9, s. 2411–2421.
  33. Kulbacka J., Poła A., Mosiądz D., Choromańska A., Nowak P.M., Kotulska M., Majkowski M., Hryniewicz-Jankowska A., Purzyc L., Saczko J.: *Cyanines as effi-*

- cient photosensitizers in photodynamic reaction: photophysical properties and in vitro photodynamic activity.* Biochemistry (Moscow). 2011, Vol. 76, No. 4, s. 473–476.
34. Langner K.M., Janowski T., Góra R., Dziekoński P., Sokalski A., Pulay P.: *The ethidium–UA/AU intercalation site: effect of model fragmentation and backbone charge state.* Journal of Chemical Theory and Computation. 2011, Vol. 7, No. 8, s. 2600–2609.
35. Lodola A., Capoferri L., Rivara S., Chudyk E., Sirirak J., Dyguda-Kazimierowicz E.B., Sokalski A., Mileni M., Tarzia G., Piomelli D., Mor M., Mulholland A.J.: *Understanding the role of carbamate reactivity in fatty acid amide hydrolase inhibition by QM/MM mechanistic modelling.* Chemical Communications. 2011, Vol. 47, s. 2517–2519.
36. Lodowski P., Jaworska M., Kornobis K., Andruniów T., Kozłowski P.M.: *Electronic and structural properties of low-lying excited states of vitamin B12.* Journal of Physical Chemistry B. 2011, Vol. 115, No. 45, s. 13304–13319.
37. Lutsyk P., Janus K., Sworakowski J., Generali G., Capelli R., Muccini M.: *Photo-switching of an n-type organic field effect transistor by a reversible photochromic reaction in the dielectric film.* Journal of Physical Chemistry C. 2011, Vol. 115, No. 7, s. 3106–3114.
38. Majumdar D., Roszak S., Leszczynski J.: *Probing the structures and thermodynamic characteristics of the environment polluting mercuric halides, cyanides and thiocyanates.* Chemical Physics Letters. 2011, Vol. 501, No. 4–6, s. 308–314.
39. Miniewicz A., Palewska K., Sznitko L., Lipiński J.: *Single- and two-photon excited fluorescence in organic nonlinear optical single crystal 3-(1,1-Dicyanoethenyl)-1-phenyl-4,5-dihydro-1H-pyrazole.* Journal of Physical Chemistry A. 2011, Vol. 115, No. 39, s. 10689–10697.
40. Myśliwiec J., Czajkowski M., Bartkiewicz S., Żygadło K., Galewski Z., Sahraoui B.: *Influence of temperature on dynamics of birefringence switching in photochromic nematic phase.* Journal of Applied Physics. 2011, Vol. 110, No. 11, s. 113104(1–5).
41. Myśliwiec J., Czajkowski M., Bartkiewicz S., Żygadło K., Galewski Z., Sahraoui B.: *Pulsed laser induced switching of birefringence in nematic phase of photochromic molecules.* Applied Physics Letters. 2011, Vol. 98, No. 8, s. 081105(1–3).
42. Myśliwiec J., Czajkowski M., Miniewicz A., Bartkiewicz S., Kochalska A., Polakova L., Sedlakova Z., Nešpůrek S.: *Dynamics of photoinduced motions in azobenzene grafted polybutadienes.* Optical Materials (Amsterdam). 2011, Vol. 33, No. 9, s. 1398–1404.

43. Myśliwiec J., Ziemińczuk M., Miniewicz A.: *Pulsed laser induced birefringence switching in a biopolymer matrix containing azo-dye molecules*. *Optical Materials* (Amsterdam). 2011, Vol. 33, No. 9, s. 1382–1386.
44. Nowakowska-Oleksy A., Cabaj J., Olech K., Sołoducho J., Roszak S.: *Comparative study of alternating low-band-gap benzothiadiazole co-oligomers*. *Journal of Fluorescence*. 2011, Vol. 21, No. 4, s. 1625–1633.
45. Nyk M.W., Wawrzyńczyk D.M., Parjaszewski K., Samoć M.: *Spectrally resolved nonlinear optical response of upconversion lanthanide-doped NaYF<sub>4</sub> nanoparticles*. *Journal of Physical Chemistry C*. 2011, Vol. 115, No. 34, s. 16849–16855.
46. Olesiak-Bańska J., Mojzisoava H., Chauvat D., Zielinski M., Matczyszyn K., Tauc P., Zyss J.: *Liquid crystal phases of DNA: evaluation of DNA organization by two-photon fluorescence microscopy and polarization analysis*. *Biopolymers*. 2011, Vol. 95, No. 6, s. 365–375.
47. Olesiak-Bańska J., Nyk M.W., Kaczmarek D., Matczyszyn K., Pawlik K., Samoć M.: *Synthesis and optical properties of water-soluble fluoride nanophosphors co-doped with Eu<sup>3+</sup> and Tb<sup>3+</sup>*. *Optical Materials* (Amsterdam). 2011, Vol. 33, No. 9, s. 1419–1423.
48. Palewska K., Sworakowski J., Lipiński J., Nešpůrek S.: *Effect of electric permittivity of the solvent on aggregation process of the water-soluble sulfonated metal phthalocyanines*. *Journal of Photochemistry and Photobiology. A, Chemistry*. 2011, Vol. 223, No. 2/3, s. 149–156.
49. Pielak K.K., Turowska-Tyrk I., Drozd M., Szostak M.M.: *Polymorphism and cold crystallization in optically nonlinear N-benzyl-2-methyl-4-nitroaniline crystal studied by X-ray diffraction, calorimetry and Raman spectroscopy*. *Journal of Molecular Structure*. 2011, Vol. 991, No. 1–3, s. 42–49.
50. Reis H., Avramopoulos A., Loboda O., Papadopoulos M.G., Kirtman B., Luis J.M., Zalesny R.: *Electronic and vibrational, linear and nonlinear polarizabilities of Li@C<sub>60</sub> and [Li@C<sub>60</sub>]<sup>+</sup>*. *Journal of Computational Chemistry*. 2011, Vol. 32, No. 5, s. 908–914.
51. Roszak R., Trzeciak A.M., Pernak J., Borucka N.: *Effect of chiral ionic liquids on palladium-catalyzed Heck arylation of 2,3-dihydrofuran*. *Applied Catalysis A-General*. 2011, Vol. 409/410, No. 1/2, s. 148–155.
52. Roztoczyńska A.K., Bartkowiak W.: *Many-body interactions and the electric response of hydrogen-bonded molecular chains*. *Computational and Theoretical Chemistry*. 2011, Vol. 967, No. 1, s. 120–128.

53. Roztoczyńska A.K., Kaczmarek-Kędziera A., Bartkowiak W.: *Assessment of DFT functionals for the calculation of interaction-induced electric properties of molecular complexes*. Chemical Physics Letters. 2011, Vol. 503, No. 1–3, s. 39–44.
54. Roztoczyńska A.K., Kaczmarek-Kędziera A., Bartkowiak W.: *Erratum to “Assessment of DFT functionals for the calculation of interaction-induced electric properties of molecular complexes”* [Chem. Phys. Lett. 503 (2011) 39]. Chemical Physics Letters. 2011, Vol. 510, No. 1–3, s. 161–164.
55. Sahraoui B., Anczykowska A., Bartkiewicz S., Myśliwiec J.: *Optimization of liquid crystal structures for real time holography applications*. Optics Express. 2011, Vol. 19, No. 24, s. 24454–24459.
56. Saloni J., Kadłubański P., Roszak S., Majumdar D., Hill G. Jr, Leszczynski J.: *The evolution of bonding and thermodynamic properties of boron-doped small carbon clusters: an ab initio study*. ChemPhysChem. 2011, Vol. 12, No. 7, s. 1358–1366.
57. Saloni J., Lipkowski P., Dasary S.S.R., Anjaneyulu Y., Yu H., Hill G. Jr: *Theoretical study of molecular interactions of TNT, acrylic acid, and ethylene glycol dimethacrylate – elements of molecularly imprinted polymer modeling process*. Polymer. 2011, Vol. 52, No. 4, s. 1206–1216.
58. Samoć M., Corkery C.T., McDonagh A.M., Cifuentes M.P., Humphrey M.G.: *Organometallic complexes for non-linear optics. [Pt.] 49, Third-order non-linear optical spectral dependence studies of arylalkynylruthenium dendrimers*. Australian Journal of Chemistry. 2011, Vol. 64, No. 9, s. 1269–1273.
59. Samoć M.: *Third-order nonlinear optical materials: practical issues and theoretical challenges*. Journal of Molecular Modeling. 2011, Vol. 17, No. 9, s. 2183–2189.
60. Schwich T., Cifuentes Marie P., Gugger P.A., Samoć M., Humphrey M.G.: *Electronic, molecular weight, molecular volume, and financial cost-scaling and comparison of two-photon absorption efficiency in disparate molecules (organometallic complexes for nonlinear optics. 48.) – a response to Comment on Organometallic complexes for nonlinear optics. 45. Dispersion of the third-order nonlinear optical properties of triphenylamine-cored alkynylruthenium dendrimers. Increasing the nonlinear response by two orders of magnitude*. Advanced Materials (Weinheim). 2011, Vol. 23, No. 12, s. 1433–1435.
61. Siedlecka R., Turowska-Tyrk I.: *Easy and efficient deracemization of all trans-1,3-diphenyl-2,4-bis-[ $\alpha$ -hydroxybenzyl]-cyclobutane and its bisphenylsulfanyl derivative and the assignment of the absolute configuration*. Tetrahedron: Asymmetry. 2011, Vol. 22, No. 16/17, s. 1662–1666.
62. Skwara B., Góra R., Zalesny R., Lipkowski P., Bartkowiak W., Reis H., Papadopoulos M.G., Luis J.M., Kirtman B.: *Electronic structure, bonding, spectra, and*

- linear and nonlinear electric properties of Ti@C28*. Journal of Physical Chemistry A. 2011, Vol. 115, No. 37, s. 10370–10381.
63. Sworakowski J., Lutsyk P.: *Bistable organic materials in optoelectrical switches: two-electrode devices vs organic field effect transistors*. Ukrainian Journal of Physics. 2011, Vol. 56, No. 10, s. 1021–1029.
64. Szarek P., Komorowski L.: *Modeling the electron density kernels*. Journal of Computational Chemistry. 2011, Vol. 32, No. 8, s. 1721–1724.
65. Szeftczyk B., Cordeiro M.N.D.S.: *Physical properties at the base for the development of an all-atom force field for ethylene glycol*. Journal of Physical Chemistry B. 2011, Vol. 115, No. 12, s. 3013–3019.
66. Szeremeta J., Nyk M.W., Chyla A., Stręk W., Samoć M.: *Enhancement of photoconduction in a conjugated polymer through doping with copper nanoparticles*. Optical Materials (Amsterdam). 2011, Vol. 33, No. 9, s. 1372–1376.
67. Sznitko L., Myśliwiec J., Karpiniński P., Palewska K., Parafiniuk K., Bartkiewicz S., Rau I., Kajzar F., Miniewicz A.: *Biopolymer based system doped with nonlinear optical dye as a medium for amplified spontaneous emission and lasing*. Applied Physics Letters. 2011, Vol. 99, No. 3, s. 031107(1–3).
68. Sznitko L., Myśliwiec J., Parafiniuk K., Szukalski A., Palewska K., Bartkiewicz S., Miniewicz A.: *Amplified spontaneous emission in polymethyl methacrylate doped with 3-(1,1-dicyanoethenyl)-1-phenyl-4,5-dihydro-1H-pyrazole (DCNP)*. Chemical Physics Letters. 2011, Vol. 512, No. 4–6, s. 247–250.
69. Szostak M.M., Chojnacki H., Piela K.K., Okwieka U., Bidzińska E., Dyrek K.: *Helical superstructure and charged polarons contributions to optical nonlinearity of 2-methyl-4-nitroaniline crystals studied by resonance Raman, electron paramagnetic resonance, circular dichroism spectroscopies, and quantum chemical calculations*. Journal of Physical Chemistry A. 2011, Vol. 115, No. 26, s. 7448–7455.
70. Szostak M.M., Chojnacki H.: *Charged polaron-enhanced circular dichroism of optically nonlinear 3-nitroaniline crystal*. Optical Materials (Amsterdam). 2011, Vol. 33, No. 9, s. 1395–1397.
71. Turowska-Tyrk I., Kang S.-J., Scheidt W.R.: *Conformational distortions of  $\pi$ -cation radical ( $\beta$ -oxoporphyrin)copper(II) derivatives: [Cu(2,7,12-trioxoOEHP<sup>+</sup>)] [SbCl<sub>6</sub><sup>-</sup>] and [Cu(2,7-dioxoOEiBC<sup>+</sup>)] [SbCl<sub>6</sub><sup>-</sup>]*. Journal of Porphyrins and Phthalocyanines. 2011, Vol. 15, No. 5, s. 373–381.
72. Vivas M.G., Da Silva D., De Boni L., Zaleśny R., Bartkowiak W., Mendonca C.R.: *Two-photon absorption spectra of carotenoids compounds*. Journal of Applied Physics. 2011, Vol. 109, No. 10, s. 103529(1–8).

73. Wilk K., Laska U., Zielińska K., Olszowski A.: *Fluorescence probe studies upon microenvironment characteristics and aggregation properties of gemini sugar surfactants in an aquatic environment*. Journal of Photochemistry and Photobiology. A. 2011, Vol. 219, No. 2/3, s. 204–210.
74. Zoń J., Videnova-Adrabińska V., Janczak J., Wilk-Kozubek M.M., Samoć A., Gancarz R., Samoć M.: *Design, synthesis and noncentrosymmetric solid state organization of three novel pyridylphosphonic acids*. CrystEngComm. 2011, Vol. 13, No. 10, s. 3474–3484.

## 2010

1. Bąkowicz J.B., Turowska-Tyrk I.: *Crystal structures of N-(4-butyryl-3-hydroxyphenyl)acetamide monohydrate and 4-(4-chlorophenyl)-2-methyl-4-oxobutanoic acid: possibilities of Yang photocyclization*. Journal of Chemical Crystallography. 2010, Vol. 40, No. 11, s. 1021–1023.
2. Bąkowicz J.B., Turowska-Tyrk I.: *Monitoring structural transformations in crystals. [Pt.] 13, On photocyclization in 2,3,4,5,6-pentamethylbenzophenone, 1,3-diphenylbutan-1-one and 2,4,6-triisopropyl-4'-methoxybenzophenone*. Acta Crystallographica. C. 2010, Vol. 66, pt. 1, s. 29–32.
3. Baranowska A., Roztoczyńska A.K., Fernández B., Bartkowiak W., Kędziera D., Kaczmarek-Kędziera A.: *Interaction-induced electric properties and cooperative effects in model systems*. Physical Chemistry Chemical Physics. 2010, Vol. 12, s. 852–862.
4. Barillé R., Samoć A., Samoć M., Luther-Davies B., Nunzi J.-M.: *Stable frequency doubling by all-optical poling in dye-doped polymer optical fibers*. Optics Letters. 2010, Vol. 35, No. 21, s. 3595–3597.
5. Bartkowiak W., Strasburger K.: *Linear and nonlinear electric properties of spatially confined LiH molecule, studied with the finite field method*. Journal of Molecular Structure. Theochem. 2010, Vol. 960, No. 1–3, s. 93–97.
6. Bednarkiewicz A., Nyk M.W., Samoć M., Stręk W.: *Up-conversion FRET from  $Er^{3+}/Yb^{3+}:NaYF_4$  nanophosphor to CdSe quantum dots*. Journal of Physical Chemistry C. 2010, Vol. 114, No. 41, s. 17535–17541.
7. Bezugly V., Wielgus P., Kohout M., Wagner F.R.: *Electron localizability indicators ELI-D and ELIA for highly correlated wavefunctions of homonuclear dimers.  $JR\backslash O'3\_Li_2, Be_2, B_2,$  and  $C_2$* . Journal of Computational Chemistry. 2010, Vol. 31, No. 7, s. 1504–1519.

8. Bezugly V., Wielgus P., Kohout M., Wagner F.R.: *Electron localizability indicators ELI-D and ELIA for highly correlated wavefunctions of homonuclear dimers. [Pt. 2], N<sub>2</sub>, O<sub>2</sub>, F<sub>2</sub>, and Ne<sub>2</sub>/Viktor Bezugly [i in.]*. Journal of Computational Chemistry. 2010, Vol. 31, No. 12, s. 2273–2285.
9. Coe B.J., Fielden J., Foxon S.P., Brunschwig B.S., Asselberghs I., Clays K., Samoć A., Samoć M.: *Combining very large quadratic and cubic nonlinear optical responses in extended, tris-chelate metallochromophores with six  $\pi$ -conjugated pyridinium substituents*. Journal of the American Chemical Society. 2010, Vol. 132, No. 10, s. 3496–3513.
10. Coe B.J., Fielden J., Foxon S.P., Helliwell M., Brunschwig B.S., Asselberghs I., Clays K., Olesiak-Bańska J., Matczyszyn K., Samoć M.: *Quadratic and cubic nonlinear optical properties of salts of diquat-based chromophores with diphenylamino substituents*. Journal of Physical Chemistry A. 2010, Vol. 114, No. 45, s. 12028–12041.
11. Ćwikowska M., Pruchnik F.P., Starosta R., Chojnacki H., Wilczok A., Ułaszewski S.: *Dinuclear Rh(II) complexes with one polypyridyl ligand, structure, properties and antitumor activity*. Inorganica Chimica Acta. 2010, Vol. 363, No. 11, s. 2401–2408.
12. Czyżnikowska Ż., Góra R., Zalesny R., Lipkowski P., Jarzemska K.N., Dominiak P.M., Leszczynski J.: *Structural variability and the nature of intermolecular interactions in Watson – Crick B-DNA base pairs*. Journal of Physical Chemistry B. 2010, Vol. 114, No. 29, s. 9629–9644.
13. Da Silva D., Schab-Balcerzak E., Miniewicz A.: *Grating translation technique as a tool for monitoring phase shifts during holographic recording in azo-polymers*. Journal of Applied Physics. 2010, Vol. 108, No. 8, s. 083540(1–9).
14. Damczyk J., Ostasiewicz K., Radosiński Ł., Radosz A.: *Asymmetry driven phase transformations*. Acta Physica Polonica A. 2010, Vol. 118, No. 4, s. 527–530.
15. Damczyk J., Ostasiewicz K., Radosiński Ł., Radosz A.: *Asymmetry induced phase transformations*. Journal of Physics (Conference Series). 2010, Vol. 213, No. 1, s. 012026(1–7).
16. Dyonizy A., Nowak P.M., Mora C., Król-Gracz A., Michalak E.: *Tabular silver halide crystals prepared by controlled Ostwald growth in the presence of dimethyl sulphoxide*. Crystal Research and Technology. 2010, Vol. 45, No. 3, s. 226–232.
17. Dyonizy A., Nowak P.M.: *Morphology of silver bromide crystals produced at presence of N,N -dimethylformamide*. Crystal Research and Technology. 2010, Vol. 45, No. 8, s. 811–816.

18. Dyonizy A., Nowak P.M.: *Obtaining tabular silver bromide crystals using double-jet method in the presence of dimethyl sulfoxide*. *Crystal Research and Technology*. 2010, Vol. 45, No. 11, s. 1171–1178.
19. Humphrey M.G., Cifuentes M.P., Samoć M.: *NLO molecules and materials based on organometallics: cubic NLO properties*. *Topics in Organometallic Chemistry*. 2010, Vol. 28, s. 57–73.
20. Janik R., Kucharski S., Sobolewska A.M., Barillé R.: *Chemical modification of glass surface with a monolayer of nonchromophoric and chromophoric methacrylate terpolymer*. *Applied Surface Science*. 2010, Vol. 257, No. 3, s. 861–866.
21. Jeffery C.J., Cifuentes M.P., Dalton G.T., Corkery C.T., Randles M.D., Willis A.C., Samoć M., Humphrey M.G.: *Organometallic complexes for nonlinear optics, 47 – synthesis and cubic optical nonlinearity of a stilbenylethynylruthenium dendrimer*. *Macromolecular Rapid Communications*. 2010, Vol. 31, No. 9/10 (spec.), s. 846–849.
22. Kuchta B., Firlej L., Roszak S., Pfeifer P., Wexler C.: *Influence of structural heterogeneity of nanoporous sorbent walls on hydrogen storage*. *Applied Surface Science*. 2010, Vol. 256, No. 17, s. 5270–5274.
23. Kuchta B., Firlej L., Roszak S., Pfeifer P.: *A review of boron enhanced nanoporous carbons for hydrogen adsorption: numerical perspective*. *Adsorption*. 2010, Vol. 16, No. 4/5, s. 413–421.
24. Kuriata-Adamusiak R., Gajcy K., Turowska-Tyrk I., Lochyński S.: *Stereochemistry of terpene derivatives. Pt. 6, Chemoenzymatic synthesis of chiral bicyclo[3.1.0]hexane derivatives with olfactory properties*. *Tetrahedron: Asymmetry*. 2010, Vol. 21, No. 7, s. 805–809.
25. Lutsyk P., Janus K., Mikołajczyk M., Sworakowski J., Boratyński B., Tłaczała M.: *Long-lived persistent currents in poly(3-octylthiophene) thin film transistors*. *Organic Electronics*. 2010, Vol. 11, No. 3, s. 490–497.
26. Lutsyk P., Sworakowski J., Janus K., Nešpůrek S., Kochalska A.: *Photochromic systems as models for opto-electrical switches*. *Molecular Crystals and Liquid Crystals*. 2010, Vol. 522, s. 211–228.
27. Majumdar D., Roszak S., Leszczynski J.: *Density functional theory based studies on the nature of Raman and resonance Raman scattering of nerve agent bound to gold and oxide-supported gold clusters: a plausible way of detection*. *Journal of Physical Chemistry A*. 2010, Vol. 114, No. 12, s. 4340–4353.

28. Mikołajczyk M., Toman P., Bartkowiak W.: *Theoretical modeling of influence of the structural disorder on the charge carrier mobility in triphenylene stacks*. Chemical Physics Letters. 2010, Vol. 485, No. 1–3, s. 253–257.
29. Mossakowska I., Wójcik G.: *Supramolecular assemblies of single-substituted nitrobenzenes in their experimental and predicted crystal structures*. Journal of Molecular Structure. 2010, Vol. 967, No. 1–3, s. 119–130.
30. Myśliwiec J., Sznitko L., Sobolewska A.M., Bartkiewicz S., Miniewicz A.: *Lasing effect in a hybrid dye-doped biopolymer and photochromic polymer system*. Applied Physics Letters. 2010, Vol. 96, No. 14, s. 141106(1–3).
31. Neshev D.N., Dreischuh A., Maleshkov G., Samoć M., Kivshar Y.S.: *Supercontinuum generation with optical vortices*. Optics Express. 2010, Vol. 18, No. 17, s. 18368–18373.
32. Nešpůrek S., Kochalska A., Nožár J., Kadashchuk A., Fishchuk I.I., Sworakowski J., Kajzar F.: *Feature of polaronic charge carriers in polysilanes: experimental and theoretical approach*. Molecular Crystals and Liquid Crystals. 2010, Vol. 521, s. 72–83.
33. Nyk M.W., Palewska K., Kępiński L., Wilk K., Stręk W., Samoć M.: *Fluorescence resonance energy transfer in a non-conjugated system of CdSe quantum dots/zinc-phthalocyanine*. Journal of Luminescence. 2010, Vol. 130, No. 12, s. 2487–2490.
34. Pawlik G., Mituś A., Myśliwiec J., Miniewicz A., Grote J.G.: *Photochromic dye semi-intercalation into DNA-based polymeric matrix: computer modeling and experiment*. Chemical Physics Letters. 2010, Vol. 484, No. 4–6, s. 321–323.
35. Radośniński Ł., Nasu K., Luty T., Radosz A.: *Possible domain-type collective dimerization of graphite induced by interlayer charge transfer excitations in the visible region*. Physical Review. B, Condensed Matter and Materials Physics. 2010, Vol. 81, No. 3, s. 035417(1–6).
36. Saloni J., Kołodziejczyk W., Roszak S., Majumdar D., Hill G., Leszczynski J.: *Local and global electronic effects in single and double boron-doped carbon nanotubes*. Journal of Physical Chemistry C. 2010, Vol. 114, No. 3, s. 1528–1533.
37. Schapiro I., Ryazantsev M.N., Ding W.J., Huntress M.M., Melaccio F., Andruniów T., Olivucci M.: *Computational photobiology and beyond*. Australian Journal of Chemistry. 2010, Vol. 63, No. 3, s. 413–429.
38. Sobolewska A.M., Bartkiewicz S., Miniewicz A., Schab-Balcerzak E.: *Polarization dependence of holographic grating recording in azobenzene-functionalized*

- polymers monitored by visible and infrared light*. Journal of Physical Chemistry B. 2010, Vol. 114, No. 30, s. 9751–9760.
39. Soras G., Psaroudakis N., Mousdis G.A., Manos M.J., Tasiopoulos A.J., Aloukos P., Couris S., Labéguerie P., Lipiński J., Avramopoulos A., Papadopoulos M.: *Synthesis and non-linear optical properties of some novel nickel derivatives*. Chemical Physics. 2010, Vol. 372, No. 1–3, s. 33–45.
  40. Szarek P., Watanabe K., Ichikawa K., Tachibana A.: *Electronic stress tensor study of aluminum nanostructures for hydrogen storage*. Materials Science Forum. 2010, Vol. 638–642, s. 1137–1142.
  41. Szefczyk B., Franco R., Gomes J.N.F., Cordeiro M.N.D.S.: *Structure of the interface between water and self-assembled monolayers of neutral, anionic and cationic alkane thiols*. Journal of Molecular Structure. Theochem. 2010, Vol. 946, No. 1–3, s. 83–87.
  42. Sznitko L., Anczykowska A., Myśliwiec J., Bartkiewicz S.: *Influence of grating period on kinetics of self-diffraction in nematic liquid crystal panel with photoconducting polymeric layer*. Applied Physics Letters. 2010, Vol. 96, No. 11, s. 111106(1–3).
  43. Trzebiatowska-Gusowska M., Piela K.K., Misiaszek T., Szostak M.M., Baran J.: *The revision of intermolecular interactions in 1,3-dinitrobenzene crystal – the role of nitro groups in optical nonlinearity*. Journal of Raman Spectroscopy. 2010, Vol. 41, No. 10, s. 1338–1347.
  44. Vivas M.G., Da Silva D., Misoguti L., Zalesny R., Bartkowiak W., Mendonca C.R.: *Degenerate two-photon absorption in all-trans retinal: nonlinear spectrum and theoretical calculations*. Journal of Physical Chemistry A. 2010, Vol. 114, No. 10, s. 3466–3470.
  45. Wexler C., Olsen R., Pfeifer P., Kuchta B., Firlej L., Roszak S.: *Numerical analysis of hydrogen storage in carbon nanopores*. International Journal of Modern Physics B. 2010, Vol. 24, No. 25/26, s. 5152–5162.
  46. Wiśniewski Ł., Deperasińska I., Staszewska A., Stefanowicz P., Berski S., Lipkowski P., Szewczuk Z., Szemik-Hojniak A.: *Photophysical properties of dipeptides containing substituted 3-(quinoxalin-6-yl) alanine: spectroscopic studies and theoretical calculations*. Journal of Physical Chemistry A. 2010, Vol. 114, No. 35, s. 9405–9412.
  47. Wojaczyńska E., Zielińska-Błajet M., Turowska-Tyrk I., Skarżewski J.: *Sulfoxides derived from Cinchona alkaloids – chiral ligands in palladium-catalyzed asymmetric allylic alkylation*. Tetrahedron: Asymmetry. 2010, Vol. 21, No. 7, s. 853–858.

48. Zaleśny R., Bulik I., Bartkowiak W., Luis J.M., Avramopoulos A., Papadopoulos M.G., Krawczyk P.: *Electronic and vibrational contributions to first hyperpolarizability of donor-acceptor substituted azobenzene*. Journal of Chemical Physics. 2010, Vol. 133, No. 24, s. 244308(1–7).
49. Zaleśny R., Loboda O., Iliopoulos K., Chatzikyriakos G., Couris S., Rotas G., Tagmatarchis N., Avramopoulos A., Papadopoulos M.G.: *Linear and nonlinear optical properties of triphenylamine-functionalized C<sub>60</sub>: insights from theory and experiment*. Physical Chemistry Chemical Physics. 2010, Vol. 12, s. 373–381.
50. Zhang C., Matsumoto T., Samoć M., Petrie S., Meng S., Corkery C.T., Stranger R., Zhang J., Humphrey M.G., Tatsumi K.: *Dodecanuclear-ellipse and decanuclear-wheel nickel(II) thiolato clusters with efficient femtosecond nonlinear absorption*. Angewandte Chemie (Int. ed.). 2010, Vol. 49, No. 25, s. 4209–4212.

## 2009

1. Andruniów T., Jaworska M., Lodowski P., Zgierski M.Z., Dreos R., Randaccio L., Kozłowski P.M.: *Time-dependent density functional theory study of cobalt corrinoids: electronically excited states of coenzyme B12*. Journal of Chemical Physics. 2009, Vol. 131, No. 10, s. 105105(1–15).
2. Andruniów T., Olivucci M.: *How does the relocation of internal water affect resonance Raman spectra of rhodopsin?: an insight from CASSCF/Amber calculations*. Journal of Chemical Theory and Computation. 2009, Vol. 5, No. 11, s. 3096–3104.
3. Babgi B., Rigamonti L., Cifuentes M.P., Corkery C.T., Randles M.D., Schwich T., Petrie S., Stranger R., Teshome A., Asselberghs I., Clays K., Samoć M., Humphrey M.G.: *Length-dependent convergence and saturation behavior of electrochemical, linear optical, quadratic nonlinear optical, and cubic nonlinear optical properties of dipolar alkynylruthenium complexes with oligo(phenyleneethynylene) bridges*. Journal of the American Chemical Society. 2009, Vol. 131, No. 29, s. 10293–10307.
4. Bąkiewicz J.B., Turowska-Tyrk I.: *2-Oxo-2-phenyl-N-[(R)-1-phenylethyl]acetamide and N,N-dimethyl-2-(1-naphthyl)-2-oxoacetamid: possibility of Yang photocyclization in a crystal*. Acta Crystallographica. C. 2009, Vol. 65, pt. 8, s. 377–380.
5. Cabaj J., Chyla A., Sołoducho J.: *Thin protein LB films as functional components within biosensors*. Materials Science-Poland. 2009, Vol. 27, No. 3, s. 685–692.
6. Cabaj J., Sołoducho J., Chyla A., Bryjak J., Labus K.T.: *The characterization of ordered thin films built of immobilized phenoloxidases*. Sensors and Actuators. B. 2009, Vol. 136, No. 2, s. 425–431.

7. Chojnacki H., Kuduk-Jaworska J., Jaroszewicz I., Jański J.J.: *Non-empirical-quantum chemical studies on hydration of trans- and cis-[Pt(NH<sub>3</sub>)<sub>2</sub>Cl<sub>2</sub>]. Possible role of relativistic effects*. Polish Journal of Chemistry. 2009, Vol. 83, No. 5, s. 1013–1024.
8. Chojnacki H., Kuduk-Jaworska J., Jaroszewicz J., Jański J.J.: *In silico approach to cisplatin toxicity: quantum chemical studies on platinum(II)–cysteine systems*. Journal of Molecular Modeling. 2009, Vol. 15, No. 6, s. 659–664.
9. Czyżnikowska Ż., Kozłowska J.J., Zaleśny R., Lipkowski P., Bartkowiak W.: *Reinvestigation of electronic structure and electric properties of large betaine molecules: a combined long-range-corrected DFT and coupled-cluster study*. Chemical Physics Letters. 2009, Vol. 480, No. 1–3, s. 37–40.
10. Czyżnikowska Ż., Lipkowski P., Góra R., Zaleśny R., Cheng A.C.: *On the nature of intermolecular interactions in nucleic acid base-amino acid side-chain complexes*. Journal of Physical Chemistry B. 2009, Vol. 113, No. 33, s. 11511–11520.
11. Czyżnikowska Ż., Zaleśny R.: *Theoretical insights into the nature of intermolecular interactions in cytosine dimer*. Biophysical Chemistry. 2009, Vol. 139, No. 2/3, s. 137–143.
12. Da Silva D., Krawczyk P., Bartkowiak W., Mendonca C.R.: *Theoretical study of one- and two-photon absorption spectra of azoaromatic compounds*. Journal of Chemical Physics. 2009, Vol. 131, No. 24, s. 244516(1–12).
13. Dalton G.T., Cifuentes M.P., Watson L.A., Petrie S., Stranger R., Samoć M., Humphrey M.G.: *Organometallic complexes for nonlinear optics: 42.(1) Syntheses, linear, and nonlinear optical properties of ligated metal-functionalized oligo(p-phenyleneethynylene)s*. Inorganic Chemistry. 2009, Vol. 48, No. 14, s. 6534–6547.
14. Doskocz M., Sołoducho J., Cabaj J., Nowakowska-Oleksy A., Roszak S.: *Functionalized phenothiazine and carbazole chromophores: synthesis and characterization*. Phosphorus, Sulfur, and Silicon and the Related Elements. 2009, Vol. 184, No. 5, s. 1257–1268.
15. Doskocz M., Strupińska A., Roszak S., Prokopowicz M., Koole Le H., Kafarski P.: *Theoretical study of spin-spin coupling across the hydrogen (O-H/N) bond in adenosine derivatives*. Journal of Molecular Modeling. 2009, Vol. 15, No. 6, s. 651–658.
16. Firlej L., Roszak S., Kuchta B., Pfeifer P., Wexler C.: *Enhanced hydrogen adsorption in boron substituted carbon nanopores*. Journal of Chemical Physics. 2009, Vol. 131, No. 16, s. 164702(1–3).

17. Ge Q., Corkery C.T., Humphrey M.G., Samoć M., Hor A.T.S.: *Organobimetallic RuII–ReI 4-ethynylpyridyl complexes: structures and non-linear optical properties*. Dalton Transactions. 2009, No. 31, s. 6192–6200.
18. Ge Q., Dalton G.T., Humphrey M.G., Samoć M., Hor A.T.S.: *Structural and non-linear optical properties of aligned heterotrinnuclear [RuII-(spacer)-MII-(spacer)-RuII] complexes (M=Pd, Pt; spacer=4-ethynylpyridine)*. Chemistry – An Asian Journal. 2009, Vol. 4, No. 6, s. 998–1005.
19. Golebiowska M., Firlej L., Kuchta B., Fabiański R.: *Structural transformations of nitrogen adsorbed on graphite: Monte Carlo studies of spatial heterogeneity in multilayer system*. Journal of Chemical Physics. 2009, Vol. 130, No. 20, s. 204703(1–7).
20. Green K.A., Cifuentes M.P., Corkery C.T., Samoć M., Humphrey M.G.: *Switching the cubic nonlinear optical properties of an electro-, halo-, and photochromic ruthenium alkynyl complex across six states*. Angewandte Chemie (Int. Ed.). 2009, Vol. 48, No. 42, s. 7867–7870.
21. Kaczmarek A., Bartkowiak W.: *The influence of the chemical compression on the electric properties of molecular systems within the supermolecular approximation: the LiH molecule as a case study*. Physical Chemistry Chemical Physics. 2009, Vol. 11, s. 2885–2892.
22. Karpiński P., Miniewicz A.: *Investigation of enhancement of photoinduced reorientation of liquid-crystal molecules in the presence of azo-dye and gold nanoparticles*. Europhysics Letters. 2009, Vol. 88, No. 5, s. 56003(1–6).
23. Komorowski L., Lipiński J., Szarek P.: *Polarization justified Fukui functions*. Journal of Chemical Physics. 2009, Vol. 131, No. 12, s. 124120(1–9).
24. Krawczyk P., Kaczmarek A., Zaleśny R., Matczyszyn K., Bartkowiak W., Ziółkowski M., Cysewski P.: *Linear nonlinear optical properties of azobenzene derivatives*. Journal of Molecular Modeling. 2009, Vol. 15, No. 6, s. 581–590.
25. Loboda O., Zaleśny R., Avramopoulos A., Luis J.M., Kirtman B., Tagmatarchis N., Reis H., Papadopoulos M.: *Linear and nonlinear optical properties of [60]fullerene derivatives*. Journal of Physical Chemistry A. 2009, Vol. 113, No. 6, s. 1159–1170.
26. Lodowski P., Jaworska M., Andruniów T., Kumar M., Kozłowski P.M.: *Article photodissociation of Co-C bond in methyl- and ethylcobalamin: an insight from TD-DFT calculations*. Journal of Physical Chemistry B. 2009, Vol. 113, No. 19, s. 6898–6908.
27. Mojzisoava H., Olesiak-Bańska J., Zieliński M., Matczyszyn K., Chauvat D., Zyss J.: *Polarization-sensitive two-photon microscopy study of the organization of liquid-crystalline DNA*. Biophysical Journal. 2009, Vol. 97, No. 8, s. 2348–2357.

28. Myśliwiec J., Czajkowski M., Miniewicz A., Kochalska A., Sedlakova Z., Nešpůrek S.: *Grafted polybutadiene for fast retrieval of optical information*. Journal of Applied Physics. 2009, Vol. 106, No. 5, s. 0531108(1–4).
29. Myśliwiec J., Sznitko L., Bartkiewicz S., Miniewicz A., Essaidi Z., Kajzar F., Sahraoui B.: *Amplified spontaneous emission in the spiropyran-biopolymer based system*. Applied Physics Letters. 2009, Vol.94, No. 24, s. 241106(1–3).
30. Myśliwiec J., Sznitko L., Miniewicz A., Kajzar F., Sahraoui B.: *Study of the amplified spontaneous emission in a dye-doped biopolymer-based material*. Journal of Physics D. 2009, Vol. 42, No. 8, s. 1–4.
31. Okwieka U., Hołderna-Natkaniec K., Misiaszek T., Medycki W., Baran J., Szostak M.M.: *Dynamical disorder in 2-methyl-4-nitroaniline and its deuterated analogue crystals studied by Fourier transform infrared and nuclear magnetic resonance*. Journal of Chemical Physics. 2009, Vol. 131, No. 14, s. 144505(1–7).
32. Olesiak-Bañska J., Matczyszyn K., Mojzisova H., Zieliński M., Chauvat D., Zyss J.: *Liquid crystalline phases in DNA and dye-doped DNA solutions analysed by polarized linear and nonlinear microscopy and differential scanning calorimetry*. Materials Science-Poland. 2009, Vol. 27, No. 3, s. 813–823.
33. Olsztyńska-Janus S., Szyborska-Małek K., Komorowska M., Lipiński J.: *Conformational changes of l-phenylalanine – near infrared-induced mechanism of dimerization: B3LYP studies*. Journal of Molecular Structure. Theochem. 2009, Vol. 911, No. 1–3, s. 1–7.
34. Piovesan E., Da Silva D., De Boni L., Guimaraes F.E.G., Misoguti L., Zaleśny R., Bartkowiak W., Mendonca C.R.: *Two-photon absorption of perylene derivatives: Interpreting the spectral structure*. Chemical Physics Letters. 2009, Vol. 479, No. 1–3, s. 52–55.
35. Roberts R.L., Schwich T., Corkery C.T., Cifuentes M.P., Green K.A., Farmer J.D., Low P.J., Marder T.B., Samoć M., Humphrey M.G.: *Organometallic complexes for nonlinear optics: 45. Dispersion of the third-order nonlinear optical properties of triphenylamine-cored alkynylruthenium dendrimers*. Advanced Materials (Weinheim). 2009, Vol. 21, No. 22, s. 1–5.
36. Schab-Balcerzak E., Siwy M., Kawalec M., Sobolewska A.M., Chamera A.M., Miniewicz A.: *Synthesis, characterization, and study of photoinduced optical anisotropy in polyimides containing side azobenzene units*. Journal of Physical Chemistry A. 2009, Vol. 113, No. 30, s. 8765–8780.
37. Skwara B., Bartkowiak W., Da Silva D.: *On the basis set superposition error in supermolecular calculations of interaction-induced electric properties: many-body components*. Theoretical Chemistry Accounts. 2009, Vol. 122, No. 3/4, s. 127–136.

38. Sobolewska A.M., Bartkiewicz S.: *On the long time holographic grating recording process in azo-polymer*. Applied Physics Letters. 2009, Vol. 95, No. 12, s. 123302(1–3).
39. Strasburger K.: *Modified adiabatic approximation: charge asymmetry in HD<sup>+</sup> and HD* Journal of Chemical Physics. 2009, Vol. 131, No. 13, s. 134103(1–8).
40. Szefczyk B., Cordeiro M.N.D.S., Franco R., Gomes J.A.N.F.: *Molecular dynamics simulations of mouse ferrochelatase variants: what distorts and orientates the porphyrin*. Journal of Biological Inorganic Chemistry. 2009, Vol. 14, No. 7, s. 1119–1128.
41. Sznitko L., Bartkiewicz S., Anczykowska A., Myśliwiec J.: *Study of self-diffraction phenomenon in hybrid liquid crystal panel*. Journal of Physics D. 2009, Vol. 42, No. 20, s. 1–5.
42. Szostak M.M., Chojnacki H., Saryga E., Dłużniewski M., Bąk G.W.: *Contribution to molecular mechanism of optical nonlinearity and electric conductivity of 3-nitroaniline single crystals by dielectric, electric and quantum chemical studies*. Chemical Physics. 2009, Vol. 365, No. 1–2, s. 44–52.
43. Tarana M., Wielgus P., Roszak S., Fabrikant I.I.: *Effects of two vibrational modes in the dissociative electron attachment to CF<sub>3</sub>Cl*. Physical Review. A. 2009, Vol. 79, No. 5, s. 052712(1–11).
44. Toman P., Nešpůrek S., Bartkowiak W.: *Modelling of charge carrier transport in conjugated polymers doped by polar additives*. Materials Science-Poland. 2009, Vol. 27, No. 3, s. 797–812.
45. Toman P., Nešpůrek S., Weiter M., Vala M., Sworakowski J., Bartkowiak W., Mensik M.: *Model of the influence of energetic disorder on inter-chain charge carrier mobility in poly[2-methoxy-5-(2'-ethylhexyloxy)-p-phenylene vinylene]*. Polymers for Advanced Technologies. 2009, Vol. 20, No. 3, s. 263–267.
46. Zaleśny R., Wójcik G., Mossakowska I., Bartkowiak W., Avramopoulos A., Papadopoulos M.G.: *Static electronic and vibrational first hyperpolarizability of meta-dinitrobenzene as studied by quantum chemical calculations*. Journal of Molecular Structure. Theochem. 2009, Vol. 907, s. 46–50.

## 2008

1. Andruniów T., Jaworska M., Lodowski P., Zgierski M.Z., Dreos R., Randaccio L., Kozłowski P.M.: *Time-dependent density functional theory study of cobalt corrinoids: electronically excited states of methylcobalamin*. Journal of Chemical Physics. 2008, Vol. 129, No. 8, s. 085101(1–14).

2. Bąkowicz J.B., Turowska-Tyrk I.: *rac-3-Benzoyl-2-methylproppionic acid and organic salts: possibilities of Yang photocyclization in crystals*. Acta Crystallographica. C. 2008, Vol. 64, pt. 8, s. 437–440.
3. Boratyński P., Turowska-Tyrk I., Skarżewski J.: *Stereoselective C9 carbon-carbon couplings of quinine: Synthesis and conformational analysis of new C2-symmetric dimers*. Journal of Organic Chemistry. 2008, Vol. 73, No. 18, s. 7357–7360.
4. Boratyński P., Turowska-Tyrk I., Skarżewski J.: *Stereoselective C9 arylation and vinylation of Cinchona alkaloids*. Organic Letters. 2008, Vol. 10, No. 3, s. 385–388.
5. Borisenko V., Krekov S., Fomenko M., Koll A., Lipkowski P.: *Influence of methoxy- and nitro-substitutions in the aromatic ring on proton donation ability in hydrogen bond and on the amino group parametrs of free and H-bonded molecules of 2-aminopyrimidine*. Journal of Molecular Structure. 2008, Vol. 882, No. 1–3, s. 9–23.
6. Cabaj J., Idzik K., Sołoducho J., Chyla A., Bryjak J., Doskocz J.: *Well-ordered thin films as practical components of biosensors*. Thin Solid Films. 2008, Vol. 516, No. 6, s. 1171–1174.
7. Chojnacki H.: *Nondynamical correlation energy in model molecular systems*. International Journal of Quantum Chemistry. 2008, Vol. 108, No. 12, s. 2267–2271.
8. Doskocz M., Roszak S., Majumdar D., Doskocz J., Gancarz R., Leszczynski J.: *Theoretical studies on the mechanism of C-P bond cleavage of a model alfa-aminophosphonate in acidic condition*. Journal of Physical Chemistry A. 2008, Vol. 112, No. 10, s. 2077–2081.
9. Doskocz M., Roszak S., Gancarz R.: *The decomposition of alfa-aminophosphine oxides to phosphonic acid derivatives (P III)*. Journal of Molecular Modeling. 2008, Vol. 14, No. 5, s. 435–440.
10. Dyguda-Kazimierowicz E.B., Sokalski A., Leszczynski J.: *Gas-phase mechanisms of degradation of hazardous organophosphorus compounds\: do they follow a common pattern of alkaline hydrolysis reaction as in phosphotriesterase*. Journal of Physical Chemistry B. 2008, Vol. 112, No. 32, s. 9982–9991.
11. Filarowski A., Koll A., Lipkowski P., Pawlukoje A.: *Inelastic neutron scattering and vibrational spectra of 2-(N-methyl-alfa-iminoethyl)-phenol and 2-(N-methyl-iminoethyl)-phenol: Experimental and theoretical approach*. Journal of Molecular Structure. 2008, Vol. 880, No. 1–3, s. 97–108.
12. Kaczorowski D., Nyk M.W., Gluchowski P., Stręk W.: *Magnetic behavior of Gd-doped GaN nanoceramics*. Journal of Alloys and Compounds. 2008, Vol. 451, No. 1–2, s. 500–503.

13. Kluba M., Lipkowski P., Filarowski A.: *Theoretical investigation of tautomeric equilibrium in ortho-hydroxy phenyl Schiff bases*. Chemical Physics Letters. 2008, Vol. 463, No. 4–6, s. 426–430.
14. Kratochvílová I., Nešpůrek S., Šebera J., Záliš S., Pavelka M., Wang G., Sworakowski J.: *New organic FET-like photoactive device, experiments and DFT modeling*. European Physical Journal. E, Soft Matter. 2008, Vol. 25, No. 3, s. 299–307.
15. Kropidłowska A., Turowska-Tyrk I., Becker B.: *Chlorido(ethyldiphenylphosphine-kappa P)(1-pyrrolidinecarbodithioato-kappa S-2,S') nickel(II)*. Acta Crystallographica. E. 2008, Vol. E64, s. 748.
16. Lewanowicz A., Gancarz R.: *An intermolecular hydrogen transfer process inducing triplet biradical photochromism of 1-methyl-2,4,4,6-tetraphenyl-1,4-dihydropyridine in the solid state*. Journal of Photochemistry and Photobiology A. 2008, Vol. 196, No. 1, s. 59–66.
17. Lis S.M., Dylewicz R., Myśliwiec J., Miniewicz A., Patela S.: *Application of flowable oxides in photonics*. Materials Science-Poland. 2008, Vol. 26, No. 1, s. 189–194.
18. Matczyszyn K., Chwiałkowska A., Sworakowski J.: *Photochromic reaction-induced changes of ordering in liquid crystalline films*. Thin Solid Films. 2008, Vol. 516, No. 24, s. 8899–8904.
19. Miniewicz A., Myśliwiec J., Pawlaczyk P., Zieliński M.: *Photorefractive-like all-optical switching in nematic-photoconducting polymer liquid crystal cell*. Molecular Crystals and Liquid Crystals. 2008, Vol. 489, No. 1, s. 119–134.
20. Myśliwiec J., Kochalska A., Miniewicz A.: *Biopolymer-bases material used in optical image correlation*. Applied Optics. 2008, Vol. 47, No. 11, s. 1902–1906.
21. Myśliwiec J., Miniewicz A., Rau I., Krupka O., Sahraoui B., Kajzar F., Grote J.: *Biopolymer-based material for optical phase conjugation*. Journal of Optoelectronics and Advanced Materials. 2008, Vol. 10, No. 8, s. 2146–2150.
22. Nešpůrek S., Pospisil J., Kratochvílová I., Sworakowski J.: *Polymeric composites based on polysilanes for plastic electronics*. Molecular Crystals and Liquid Crystals. 2008, Vol. 484, s. 265–290.
23. Nešpůrek S., Zmeskal O., Sworakowski J.: *Space-charge-limited currents in organic films: some open problems*. Thin Solid Films. 2008, Vol. 516, No. 24, s. 8949–8962.
24. O'Boyle N.M., Tenderholt A.L., Langner K.M.: *Cclib: a library for package-independent computational chemistry algorithms*. Journal of Computational Chemistry. 2008, Vol. 29, No. 5, s. 839–845.

25. Okwieka U., Szostak M.M., Misiaszek T., Turowska-Tyrk I., Natkaniec I., Pavluškojc A.: *Spectroscopic, structural and theoretical studies of 2-methyl-4-nitroaniline (MNA) crystal: electronic transitions in IR*. Journal of Raman Spectroscopy. 2008, Vol. 39, No. 7, s. 849–862.
26. Olsztyńska-Janus S., Szyborska-Małek K., Komorowska M., Lipiński J.: *Usefulness of spectroscopy for biomedical engineering*. Acta of Bioengineering and Biomechanics. 2008, Vol. 10, No. 3, s. 45–49.
27. Palewska K., Sujka M., Uraśńska-Wójcik B., Sworakowski J., Lipiński J., Nešpůrek S., Rakusan J., Karaskova M.: *Light-induced effects in sulfonated aluminum phthalocyanines potential photosensitizers in the photodynamic therapy: Spectroscopic and kinetic study*. Journal of Photochemistry and Photobiology A. 2008, Vol. 197, No. 1, s. 1–12.
28. Puchalska M., Turowska-Tyrk I., Trush V., Legendziewicz J.: *Structural characteristic and luminescence properties of first known example of a pair of europium(III) complexes of phosphoroazo-derivative of beta-diketone with inner and both inner and outer sphere 2,2'-bipyridine*. Journal of Alloys and Compounds. 2008, Vol. 451, No. 1/2, s. 264–269.
29. Schab-Balcerzak E., Sobolewska A.M., Miniewicz A., Jurusik J.: *Chromophore concentration effect on holographic grating formation efficiency in novel azobenzene functionalized polymers*. Polymer Engineering and Science. 2008, Vol. 48, No. 9, s. 1755–1767.
30. Schab-Balcerzak E., Sobolewska A.M., Miniewicz A.: *Comparative studies of newly synthesized azo-dyes bearing poly(esterimide)s with their poly(etherimide) analogues: light-induced optical anisotropy*. Optical Materials (Amsterdam). 2008, Vol. 31, s. 405–411.
31. Skwara B., Kaczmarek A., Góra R., Bartkowiak W.: *On decomposition of interaction-induced electric properties of HF dimer*. Chemical Physics Letters. 2008, Vol. 461, No. 4–6, s. 203–206.
32. Sobolewska A.M., Bartkiewicz S.: *Three gratings coupling during the holographic grating recording process in azobenzene-functionalized polymer*. Applied Physics Letters. 2008, Vol. 92, No. 25, s. 253305(1–3).
33. Sobolewska A.M., Miniewicz A.: *On the inscription of period and half-period surface relief gratings in azobenzene-functionalized polymers*. Journal of Physical Chemistry B. 2008, Vol. 112, No. 15, s. 4526–4535.
34. Szarek P., Dyguda-Kazimierowicz E.B., Tachibana A., Sokalski A.: *Physical nature of intermolecular interactions within cAMP-dependent protein kinase ac-*

- tive site: differential transition state stabilization in phosphoryl transfer reaction.* Journal of Physical Chemistry B. 2008, Vol. 112, No. 37, s. 11819–11826.
35. Szeftczyk B., Andruniów T., Sokalski A.: *Ab initio multireference study of Hetero-Diels-Alder reaction of buta-1,3-diene with alkyl glyoxylates.* Journal of Molecular Modeling. 2008, Vol. 14, No. 8, s. 727–733.
  36. Szeftczyk B.: *Towards understanding phosphonoacetaldehyde hydrolase: an alternative mechanism involving proton transfer that triggers P-C bond cleavage.* Chemical Communications. 2008, No. 35, s. 4162–4164.
  37. Tran V.H., Świątek-Tran B.: *Spin-glass behaviour in the coordination polymer  $[Co(C_3H_3N_2)_2]_n$ .* Dalton Transactions. 2008, No. 36, s. 4860–4865.
  38. Trzop E., Turowska-Tyrk I.: *Monitoring structural transformations in crystals: 12. Course of an intramolecular [4+4] photocycloaddition in a crystal.* Acta Crystallographica B. 2008, Vol. B64, pt. 3, s. 375–382.
  39. Wielgus P., Roszak S., Majumdar D., Saloni J., Leszczynski J.: *Theoretical studies on the bonding and thermodynamic properties of  $Ge_nSi_m$  ( $m + n = 5$ ) clusters: the precursors of germanium/silicon nanomaterials.* Journal of Chemical Physics. 2008, Vol. 128, No. 14, s. 144305(1–10).
  40. Yakunin S., Gayvoronsky V., Miniewicz A., Sworakowski J.: *Nanosecond laser pulse-induced refractive index changes in anthraquinone-doped liquid crystal.* Molecular Crystals and Liquid Crystals. 2008, Vol. 496, s. 310–321.
  41. Zaleśny R., Papadopoulos M.G., Bartkowiak W., Kaczmarek A.: *On the electron correlation effects on electronic and vibrational hyperpolarizability of merocyanine dyes.* Journal of Chemical Physics. 2008, Vol. 129, No. 13, s. 134310(1–4).
  42. Zierkiewicz W., Komorowski L., Michalska D., Cerny J., Hobza P.: *The amino group in adenine: MP2 and CCSD(T) complete basis set limit calculations of the planarization barrier and DFT/B3LYP study of the anharmonic frequencies of adenine.* Journal of Physical Chemistry B. 2008, Vol. 112, No. 51, s. 16734–16740.

## 2007

1. Allen R., Lipkowski P., Shukla M., Leszczynski J.: *Vibrational analysis of complexes of urate with IA group metal cations ( $Li^+$ ,  $Na^+$  and  $K^+$ ).* Spectrochimica Acta. A. 2007, Vol. 68, No. 4, s. 639–645.

2. Andruniów T.: *Vibrational analysis of a solvated green fluorescent protein chromophore*. Journal of Molecular Modeling, 2007, Vol. 13, No. 6/7, s. 775–783.
3. Bąkowiec J.B., Kropidłowska A., Turowska-Tyrk I., Becker B.: *mi-trans-1,2-Di-4-pyridylethene-kappa(2)N:N'-bis[(dimethylformamide-kappa(O))bis(tri-tert-butoxysilanethiolato-kappa(S))cadmium(II)]*. Acta Crystallographica. E. 2007, Vol. E63, pt. 4, s. 973–975.
4. Czyżnikowska Ż., Zaleśny R., Ziółkowski M., Góra R., Cysewski P.: *The nature of interactions in uracil dimer: an ab initio study*. Chemical Physics Letters. 2007, Vol. 450, No. 1–3, s. 132–137.
5. Doskocz J., Sołoducho J., Cabaj J., Łapkowski M., Golba S., Palewska K.: *Development in synthesis, electrochemistry, LB moieties of phenothiazine based units*. Electroanalysis. 2007, Vol. 19, No. 13, s. 1394–1401.
6. Doskocz M., Gancarz R., Roszak S.: *The protonation equilibrium and decomposition of amino- and hydroxyphosphonates, phosphine oxides and phosphonic acid*. Polish Journal of Chemistry. 2007, Vol. 81, s. 2013–2021.
7. Dyguda-Kazimierowicz E.B., Sokalski A., Leszczynski J.: *Non-empirical study of the phosphorylation reaction catalyzed by 4-methyl-5-beta-hydroxyethylthiazole kinase: relevance of the theory of intermolecular interactions*. Journal of Molecular Modeling. 2007, Vol. 13, No. 7/8, s. 839–849.
8. Dyonizy A., Nowak P.M., Mora C.: *A study of effect of agitation intensification on the size and external shape of silver bromide crystals produced by controlled ostwald growth in the presence of dimethyl sulfoxide*. Russian Journal of Applied Chemistry. 2007, Vol. 80, No. 4, s. 605–610.
9. Frutos L.M., Andruniów T., Santoro F., Ferre N., Olivucci M.: *Tracking the excited-state time evolution of the visual pigment with multiconfigurational quantum chemistry*. Proceedings of the National Academy of Sciences of the United States of America. 2007, Vol. 104, No. 19, s. 7764–7769.
10. Grabowski S.J., Sokalski A., Leszczynski J.: *Wide spectrum of H...H interactions: van der Waals contacts, dihydrogen bonds and covalency*. Chemical Physics. 2007, Vol. 333, No. 1, s. 68–76.
11. Grzywa R.K., Dyguda-Kazimierowicz E.B., Sieńczyk M., Feliks M., Sokalski A., Oleksyszyn J.: *The molecular basis of urokinase inhibition: from the nonempirical analysis of intermolecular interactions to the prediction of binding affinity*. Journal of Molecular Modeling. 2007, Vol. 13, No. 6/7, s. 677–683.
12. Jaworska M., Lodowski P., Andruniów T., Kozłowski P.M.: *Photolysis of methylcobalamin: identyfikacja of the relevant excited states involved in Co-C bond*

- scission*. Journal of Physical Chemistry B. 2007, Vol. 111, No. 10, s. 2419–2422.
13. Kaczmarek A., Zalesny R., Bartkowiak W.: *On the influence of confinement effects on electric properties: an ab initio study*. Chemical Physics Letters. 2007, Vol. 449, No. 4–6, s. 314–318.
  14. Kołodziejczyk W., Majumdar D., Roszak S., Leszczynski J.: *Probing the role of P=O stretching mode enhancement in nerve-agent sensors: simulation of the adsorption of diisopropylfluorophosphate on the model MgO and CaO surfaces*. Chemical Physics Letters. 2007, Vol. 450, No. 1–3, s. 138–143.
  15. Kropidłowska A., Turowska-Tyrk I., Becker B.: *1,3-Diethyl-1,1,3,3-tetraphenyl-disiloxane*. Acta Crystallographica. E. 2007, Vol. E63, pt. 2, s. 855–857.
  16. Langner K.M., Sokalski A., Leszczynski J.: *Intriguing relations of interaction energy components in stacked nucleic acids*. Journal of Chemical Physics. 2007, Vol. 127, No. 11, s. 111102(1–4).
  17. Lewanowicz A.: *Thermochromism of N-triphenylmethylsalicylideneimine activity of the trans-open enol conformer at low temperature*. Molecular Crystals and Liquid Crystals. 2007, Vol. 467, s. 339–351.
  18. Lumento F., Zanirato V., Fusi S., Busi E., Latterini L., Elisei F., Sinicropi A., Andruniów T., Ferre N., Basosi R., Olivucci M.: *Quantum chemical modeling and preparation of a biomimetic photochemical switch*. Angewandte Chemie (Int. Ed.). 2007, Vol. 46, No. 3, s. 414–420.
  19. Majumdar D., Roszak S., Leszczynski J.: *Do the low-energy conformers of nerve agents (NAs) really have cholinesterase inhibition properties?: investigations of the low-energy conformers of acetylcholine and the two NAs sarin and soman*. Molecular Physics. 2007, Vol. 105, No. 19–22, s. 2551–2564.
  20. Melikova S.M., Rutkowski K.S., Lipkowski P., Shchepkin D.N., Koll A.: *FTIR studies of HCl dissolved in liquid CO: Anharmonic effects in the weak OC...HCl complex*. Journal of Molecular Structure. 2007, Vol. 844–845, s. 64–69.
  21. Miniewicz A., Kochalska A., Myśliwiec J., Samoć A., Samoć M., Grote J.G.: *Deoxyribonucleic acid-based photochromic material for fast dynamic holography*. Applied Physics Letters. 2007, Vol. 91, No. 4, s. 041118(1–3).
  22. Miniewicz A., Samoć A., Samoć M., Kaszynski P.: *Observation of second-harmonic generation in an oriented glassy nematic phase of a closo-decaborane derivative*. Journal of Applied Physics. 2007, Vol. 102, No. 4, s. 033108(1–7).

23. Mossakowska I., Wójcik G: *1-Chloro-2-nitrobenzene: N-O...Cl halogen bonds and aromatic pi-pi stacking, and thermal vibrations in the vicinity of the melting point*. Acta Crystallographica. C. 2007, Vol. 63, pt. 2, s. 123–125.
24. Myśliwiec J., Bartkiewicz S., Janus K.: *Optical phase conjugation in the hybrid polymer liquid crystal panel*. Optics Communications. 2007, Vol. 276, s. 58–61.
25. Myśliwiec J., Jarzab D., Janus K., Bartkiewicz S.: *Study of self-diffraction process in photoconducting polymer-nematic liquid crystal hybrid structure*. Applied Physics Letters. 2007, Vol. 90, No. 12, s. 121120(1–3).
26. Myśliwiec J., Miniewicz A., Nešpůrek S., Studenovský M., Sedlakova Z.: *Efficient holographic recording in novel azo-containing polymer*. Optical Materials (Amsterdam). 2007, Vol. 29, No. 12, s. 1756–1762.
27. Niewodniczański W., Bartkowiak W.: *Theoretical study of geometrical and non-linear optical properties of pyridinium N-phenolate betaine dyes*. Journal of Molecular Modeling. 2007, Vol. 13, No. 6/7, s. 793–800.
28. Palewska K., Miniewicz A., Bartkiewicz S., Legendziewicz J., Stręk W.: *Influence of electric field on photoluminescence of lanthanide-doped nematic liquid crystal*. Journal of Luminescence. 2007, Vol. 124, s. 265–272.
29. Saloni J., Roszak S., Miller M., Leszczynski J.: *Thermodynamic studies of bromine-iodine competition in the formation on NaSnXYZ (X, Y, Z = Br or I) complexes*. Journal of Physical Chemistry A. 2007, Vol. 111, No. 37, s. 9139–9144.
30. Samoć A., Miniewicz A., Samoć M., Grote J.G.: *Refractive-index anisotropy and optical dispersion in films of deoxyribonucleic acid*. Journal of Applied Polymer Science. 2007, Vol. 105, s. 236–245.
31. Schab-Balcerzak E., Sobolewska A.M., Miniewicz A., Jarusik J., Jarzabek B.: *Photoinduced holographic gratings in azobenzene-functionalized poly(amideimide)s*. Polymer Journal. 2007, Vol. 39, No. 7, s. 659–669.
32. Shimizu F.M., Volpati D., Giacometti J.A., Sworakowski J., Janus K., Luboch E.: *Kinetics of photoinduced birefringence in the guest-host system of poly(methyl methacrylate) doped with azobenzene-containing crown ethers*. Journal of Applied Polymer Science. 2007, Vol. 105, s. 130–136.
33. Skwara B., Bartkowiak W., Roztoczyńska A.K., Góra R., Leszczynski J.: *On the cooperativity of the interaction-induced (hyper)polarizabilities of the selected hydrogen-bonded trimers* Chemical Physics Letters. 2007, Vol. 436, No. 1–3, s. 116–123.

34. Skwara B., Roztoczyńska A.K., Bartkowiak W.: *On the many-body components of interaction-induced electric properties: Linear fluoroacetylene trimer as a case study*. Computing Letters. 2007, Vol. 3, No. 2–4, s. 175–182.
35. Sobolewska A.M., Miniewicz A.: *Analysis of the kinetics of diffraction efficiency during the holographic grating recording in azobenzene functionalized polymers*. Journal of Physical Chemistry B. 2007, Vol. 111, No. 7, s. 1536–1544.
36. Strasburger K., Wołczyr M.: *Adiabatic method for positronic atoms and molecules*. Molecular Physics. 2007, Vol. 105, No. 4, s. 467–476.
37. Sworakowski J., Matczyszyn K.: *Non-exponential decays in first-order kinetic processes: the case of „squeezed exponential”*. Acta Physica Polonica A. 2007, Vol. 112, suppl. s. S 153–S 159.
38. Szeftczyk B., Claeysens F., Mulholland A.J., Sokalski A.: *Quantum chemical analysis of reaction paths in chorismate mutase: conformational effects and electrostatic stabilization*. International Journal of Quantum Chemistry. 2007, Vol. 107, No. 12, s. 2274–2285.
39. Szostak M.M., Kozankiewicz B., Lipiński J.: *Low-temperature photoluminescence of p-nitroaniline and o-methyl-p-nitroaniline crystals*. Spectrochimica Acta A. 2007, Vol. 67, No. 5, s. 1412–1416.
40. Turowska-Tyrk I., Bąkiewicz J.B., Scheffer J.R.: *Monitoring structural transformations in crystals: [Pt.] 11. Yang photocyclizations – one type of reaction, but diversity of structural changes*. Acta Crystallographica B. 2007, Vol. B63, pt. 6, s. 933–940.
41. Turowska-Tyrk I., Łabęcka I., Scheffer J.R., Xia W.: *Monitoring structural transformations in crystals: Pt. 10. Monitoring molecular and crystal structures during a Yang photocyclization reaction – comparative studies*. Polish Journal of Chemistry. 2007, Vol. 81, s. 813–824.
42. Vertsimakha Y., Lutsyk P., Palewska K., Sworakowski J., Lytvyn O.: *Optical and photovoltaic properties of thin films of N,N'-dimethyl-3,4,9,10-perylene-tetracarboxylic acid diimide*. Thin Solid Films. 2007, Vol. 515, No. 20/21, s. 7950–7957.
43. Wang J., Gu J., Leszczynski J., Feliks M., Sokalski A.: *Oxime-induced reactivation of sarin-inhibited AChE: a theoretical mechanisms study*. Journal of Physical Chemistry B. 2007, Vol. 111, No. 9, s. 2404–2408.
44. Wielgus P., Majumdar D., Roszak S., Leszczynski J.: *Structure and properties of the low-lying electronic states of CeC<sub>2</sub> and CeC<sub>2</sub><sup>+</sup>*. Journal of Chemical Physics. 2007, Vol. 127, No. 12, s. 124307(1–13).

45. Zaleśny R., Bartkowiak W., Toman P., Leszczynski J.: *Computational insight into relations between electronic and vibrational polarizabilities within the two-state valence-bond charge-transfer model*. Chemical Physics. 2007, Vol. 337, No. 1–3, s. 77–80.
46. Zaleśny R., Matczyszyn K., Kaczmarek A., Bartkowiak W., Cysewski P.: *Experimental and theoretical investigations of spectroscopic properties of azobenzene derivatives in solution*. Journal of Molecular Modeling. 2007, Vol. 13, No. 6/7, s. 785–791.
47. Zych T., Misiaszek T., Szostak M.M.: *Polymorphism of 2-nitroaniline studied by calorimetric (DSC), structural (X-ray diffraction) and spectroscopic (FT-IR, Raman, UV-Vis) methods*. Chemical Physics. 2007, Vol. 340, No. 1–3, s. 260–272.

## 2006

1. Almatarneh M.H., Flinn Ch.G., Poirier R., Sokalski A.: *Computational study of the deamination reaction of cytosine with H<sub>2</sub>O and OH*. Journal of Physical Chemistry A. 2006, Vol. 110, No. 26, s. 8227–8234.
2. Cabaj J., Doscocz J., Sołoducho J., Chyla A.: *Convenient synthesis and physico-chemical profile of new derivatives of pyrimidine*. Heterocycles. 2006, Vol. 68, No. 1, s. 137–149.
3. Cabaj J., Idzik K., Sołoducho J., Chyla A.: *Development in synthesis and electrochemical properties of thienyl derivatives of carbazole*. Tetrahedron. 2006, Vol. 62, No. 4, s. 758–764.
4. Cabaj J., Sołoducho J., Nowakowska-Oleksy A., Chyla A.: *Synthesis, design and electrochemical properties of Langmuir-Blodgett (LB) films built of bis(pyrrolyl)fluorene*. Electroanalysis. 2006, Vol. 18, No. 8, s. 801–806.
5. Chojnacki H., Strasburger K.: *Configuration interaction study of the positronic hydrogen cyanide molecule*. Molecular Physics. 2006, Vol. 104, No. 13/14, s. 2273–2276.
6. Doscocz M., Roszak S., Sołoducho J., Leszczynski J.: *Theoretical studies of symmetric five-membered heterocycle derivatives of carbazole and fluorene: precursors of conducting polymers*. Journal of Physical Chemistry A. 2006, Vol. 110, No. 51, s. 13989–13994.
7. Forde G.K., Kędzierski P., Sokalski A., Forde A.E., Hill G., Leszczynski J.: *Physical nature of interactions within the active site of cytosine-5-methyltransferase*. Journal of Physical Chemistry A. 2006, Vol. 110, No. 6, s. 2308–2313.

8. Fuentes-Cabrera M., Lipkowski P., Huertas O., Sumpter B.G., Orozco M., Luque F.J., Wells J.C., Leszczynski J.: *Aromaticity-induced changes in the electronic properties of size-expanded DNA bases: case of xC*. International Journal of Quantum Chemistry. 2006, Vol. 106, No. 11, s. 2339–2346.
9. Fuentes-Cabrera M., Sumpter B.G., Lipkowski P., Wells J.C.: *Size-expanded yDNA bases: an ab initio study*. Journal of Physical Chemistry B. 2006, Vol. 110, No. 12, s. 6379–6384.
10. Gayvoronsky V., Yakunin S., Pergamenschchik V., Nazarenko V., Palewska K., Sworakowski J., Podhorodecki A., Misiewicz J.: *Photoluminescence of nematic liquid crystal doped with anthraquinone dye*. Ukrainian Journal of Physical Optics. 2006, Vol. 7, No. 3, s. 116–123.
11. Godlewska P., Ban-Oganowska H., Macalik L., Hanuza J., Oganowski W., Roszak S., Lipkowski P.: *Normal coordinate analysis and DFT calculations of vibrational spectra for lanthanide(III) complexes with 3-bromo-4-methoxy-2,6-lutidine N-oxide: LnCl<sub>3</sub>(Br<sub>4</sub>CH<sub>3</sub>OC<sub>7</sub>H<sub>7</sub>NO)<sub>3</sub> (Ln = Pr, Nd, Sm, Eu, Gd, Dy)*. Journal of Molecular Structure. 2006, Vol. 782, No. 1, s. 1–15.
12. Grabowski S.J., Sadlej A.J., Sokalski A., Leszczynski J.: *Attractive halogen-halogen interactions: F<sub>3</sub>CCl...FH and F<sub>3</sub>CCl...FCH<sub>3</sub> dimers*. Chemical Physics. 2006, Vol. 327, No. 1, s. 151–158.
13. Grabowski S.J., Sokalski A., Leszczynski J.: *Can H...sigma, pi...H(+)...sigma and sigma...H(+)...sigma interactions be classified as H-bonded?*. Chemical Physics Letters. 2006, Vol. 432, s. 33–39.
14. Grabowski S.J., Sokalski A., Leszczynski J.: *Hydride bonding – ab initio studies of BeH<sub>2</sub>...Li<sup>+</sup>, BeH<sub>2</sub>...Na<sup>+</sup> and BeH<sub>2</sub>...Mg<sub>2</sub><sup>+</sup> model systems*. Chemical Physics Letters. 2006, Vol. 422, No. 4–6, s. 334–339.
15. Grabowski S.J., Sokalski A., Leszczynski J.: *The possible covalent nature of N-H...O hydrogen bonds in formamide dimer and related systems: an ab initio study*. Journal of Physical Chemistry A. 2006, Vol. 110, No. 14, s. 4772–4779.
16. Grabowski S., Sokalski A., Dyguda-Kazimierowicz E.B., Leszczynski J.: *Quantitative classification of covalent and noncovalent H-bonds*. Journal of Physical Chemistry B. 2006, Vol. 110, No. 13, s. 6444–6446.
17. Hanuza J., Mączka M., Szaśiadek W., Roszak S., Lipkowski P., Kamiński A.A., Haussuhl E., Hulliger J., Hussin A.: *Polarized IR and Raman spectra and ab initio calculations for bis(guanidine) zirconium bis(nitrilotriacetate) hydrate single crystal [C(NH<sub>2</sub>)<sub>3</sub>]<sub>2</sub>{Zr[N(CH<sub>2</sub>COO)<sub>3</sub>]<sub>2</sub>}(H<sub>2</sub>O) – the new laser Raman converter*. Spectrochimica Acta A. 2006, Vol. 65, No. 3–4, s. 969–984.

18. Jonas S., Nadachowski F., Szwagierczak D., Wójcik G.: *Thermal expansion of  $\text{CaAl}_4\text{O}_7$  – based refractory compositions containing MgO and CaO additions* Journal of the European Ceramic Society. 2006, Vol. 26, No. 12, s. 2273–2278.
19. Kozłowski P.M., Andruniów T., Jarzecki A.A., Zgierski M.Z., Spiro T.G.: *DFT analysis of Co-alkyl and Co-adenosyl vibrational modes in B12-cofactors*. Inorganic Chemistry. 2006, Vol. 45, No. 14, s. 5585–5590.
20. Kropidłowska A., Turowska-Tyrk I., Becker B.: *(2,2'-Bipyridine)bis(tri-tert-butoxysilanethiolato-k(2)O,S)cadmium(II)*. Acta Crystallographica E. 2006, Vol. E62, s. 3407–3409.
21. Langner K.M., Kędziński P., Sokalski A., Leszczynski J.: *Physical nature of ethidium and proflavine interactions with nucleic acid bases in the intercalation plane*. Journal of Physical Chemistry B. 2006, Vol. 110, No. 19, s. 9720–9727.
22. Lipkowski P., Grabowski S. J., Leszczynski J.: *Properties of the halogen-hydride interaction: an ab initio and „atoms in molecules” analysis*. Journal of Physical Chemistry A. 2006, Vol. 110, No. 34, s. 10296–10302.
23. Majumdar D., Roszak S., Leszczynski J.: *Probing the acetylcholinesterase inhibition of sarin: a comparative interaction study of the inhibitor and acetylcholine with a model enzyme cavity*. Journal of Physical Chemistry B. 2006, Vol. 110, No. 27, s. 13597–13607.
24. Miniewicz A., Myśliwiec J., Kajzar F., Parka J.: *On the real-time reconstruction of digital holograms displayed on photosensitive liquid crystal systems*. Optical Materials (Amsterdam). 2006, Vol. 28, No. 12, s. 1389–1397.
25. Miniewicz A., Sahraoui B., Schab-Balcerzak E., Sobolewska A.M., Mituś A., Kajzar F.: *Pulsed-laser grating recording in organic materials containig azobenzene derivatives*. Nonlinear Optics, Quantum Optics. 2006, Vol. 35, No. 1–3, s. 95–102.
26. Mituś A., Pawlik G., Sahraoui B., Miniewicz A., Kajzar F.: *Monte Carlo based design of photonic processes in azopolymers*. Molecular Crystals and Liquid Crystals. 2006, Vol. 446, No. 1, s. 47–54.
27. Pawlik G., Mituś A., Miniewicz A., Kajzar F.: *Computer simulations of molecular movements in functionalized polymers under spatially inhomogeneous light illumination*. Nonlinear Optics, Quantum Optics. 2006, Vol. 35, No. 1–3, s. 21–25.
28. Podolyan Y., Lipkowski P., Leszczynski J.: *A density functional theory study of vibrational infrared spectra of N-methyl-P tautomers*. Journal of Molecular Structure. 2006, Vol. 792/793, s. 9–15.

29. Saloni J., Roszak S., Hilpert K., Popovic A., Miller M., Leszczynski J.: *Mass spectrometric and quantum chemical studies of the thermodynamics and bonding of neutral and ionized LnCl, LnCl<sub>2</sub>, and LnCl<sub>3</sub> species (Ln = Ce, Lu)*. Inorganic Chemistry. 2006, Vol. 45, No. 11, s. 4508–4517.
30. Saloni J., Roszak S., Miller M., Leszczynski J.: *Theoretical thermodynamics and the nature of interactions of the quasi-binary NaCl-SnCl<sub>2</sub> system*. Journal of Physical Chemistry A. 2006, Vol. 110, No. 45, s. 12535–12539.
31. Schab-Balcerzak E., Grobelny Ł., Sobolewska A.M., Miniewicz A.: *Cycloaliphatic-aromatic polyimides based on diamines with azobenzene unit*. European Polymer Journal. 2006, Vol. 42, No. 10, s. 2859–2871.
32. Schab-Balcerzak E., Sapich B., Stumpe J., Sobolewska A.M., Miniewicz A.: *Characterization and photoinduced properties of photochromic polymers: 1. Polyesterimides with 4-amino 4'-nitro azobenzene moieties* e-Polymers. 2006, No. 021, [17], s. 11.
33. Skwara B., Bartkowiak W., Góra R., Niewodniczański W., Roszak S.: *On the weak intermolecular interactions and their influence on the optical properties of unsaturated hydrocarbons. Pt. 1, Two-body interactions*. Molecular Physics. 2006, Vol. 104, No. 13/14, s. 2263–2271.
34. Sobolewska A.M., Miniewicz A., Grabiec E., Sek D.: *Holographic grating recording in azobenzene functionalized polymers*. Central European Journal of Chemistry. 2006, Vol. 4, No. 2, s. 266–284.
35. Sworakowski J., Janus K., Nešpůrek S., Vala M.: *Local states in organic materials: charge transport and localization*. IEEE Transactions on Dielectrics and Electrical Insulation. 2006, Vol. 13, No. 5, s. 1001–1015.
36. Szeferczyk B., Kędzierski P., Sokalski A., Leszczynski J.: *Theoretical insights into catalysis by phosphonoacetaldehyde hydrolase*. Molecular Physics. 2006, Vol. 104, No. 13/14, s. 2203–2211.
37. Szymczak J.J., Góra R., Roszak S., Majumdar D., Wang J., Grabowski S.J., Leszczynski J.: *Proton bound open shell systems – theoretical studies on O<sub>2</sub>H<sup>+</sup>(O<sub>2</sub>)<sub>n</sub> (n = 1–6) complexes*. Molecular Physics. 2006, Vol. 104, No. 13/14, s. 2327–2336.
38. Szymczak J.J., Urban J., Roszak S., Leszczynski J.: *The nature of variations of ammonia proton affinity in an argon environment*. Journal of Physical Chemistry A. 2006, Vol. 110, No. 48, s. 13099–13105.
39. Turowska-Tyrk I., Bąkowicz J.B., Scheffer J.R., Xia W.: *Monitoring reaction centers and molecules during an enantioselective photoreaction in a crystal*. CrystEngComm 2006, Vol. 8, Iss. 8, s. 616–621.

40. Wielgus P., Góra R., Szeftczyk B., Roszak S., Leszczynski J.: *On the influence of microsolvation by argon atoms on the electron affinity properties of water dimer*. Journal of Chemical Physics. 2006, Vol. 124, No. 9, s. 094304(1–10).
41. Wójcik G., Holband J., Szymczak J.J., Roszak S., Leszczynski J.: *Interactions in polymorphic crystals of m-nitrophenol as studied by variable-temperature X-ray diffraction and quantum chemical calculations*. Crystal Growth & Design. 2006, Vol. 6, No. 1, s. 274–282.
42. Wójcik G., Mossakowska I.: *Polymorphs of p-nitrophenol as studied by variable-temperature X-ray diffraction and calorimetry: comparison with m-nitrophenol*. Acta Crystallographica. B. 2006, Vol. B62, Pt. 1, s. 143–152.

## 2005

1. Andruniów T., Fantacci S., De Angelis F., Ferre N., Olivucci M.: *Mechanism of the initial conformational transition of a photomodulable peptide*. Angewandte Chemie (Int. Ed.). 2005, Vol. 44, No. 37, s. 6077–6081.
2. Bartkowiak W., Lipkowski P.: *Hydrogen-bond effects on the electronic absorption spectrum and evaluation of nonlinear optical properties of an aminobenzo-difuranone derivative that exhibits the largest positive solvatochromism*. Journal of Molecular Modeling. 2005, Vol. 11, No. 4/5, s. 317–322.
3. Bartkowiak W., Niewodniczański W., Misiaszek T., Zaleśny R.: *First-order hyperpolarizability of pyridinium N-phenolate betaine dye: ab initio study*. Chemical Physics Letters. 2005, Vol. 411, No. 1–3, s. 8–13.
4. Borisenko V.E., Krekov S.A., Niyazova M.A., Koll A., Lipkowski P.: *Influence of chlorine-substitution in pyrimidine ring on proton donor ability in H-bond and parameters of amino group of 2-amino pyrimidine*. Vibrational Spectroscopy. 2005, Vol. 37, No. 1, s. 97–109.
5. Buron-Le Cointe M., Collet E., Guerin L., Lemee-Cailleau M., Cailleau H., Wulff M., Luty T., Koshihara S.Y., Tanaka K.: *Time-resolved X-ray diffraction: a wonderful tool for probing structural photo-induced phase transitions*. Journal of Luminescence. 2005, Vol. 112, No. 1–4, s. 235–241.
6. Diaz C.C., Kaplan I.G., Roszak S.: *Theoretical study of the electron affinities of the alkaline-earth tetramers possessing  $T_d$  symmetry:  $Be_4$  and  $Mg_4$* . Journal of Molecular Modeling. 2005, Vol. 11, No. 4/5, s. 330–334.
7. Dyguda-Kazimierowicz E.B., Grembecka J., Sokalski A., Leszczynski J.: *Origins of the activity of PAL and LAP enzyme inhibitors: toward ab initio binding affinity*

- prediction*. Journal of the American Chemical Society. 2005, Vol. 127, No. 6, s. 1658–1659.
8. Góra R., Grabowski S.J., Leszczynski J.: *Dimers of formic acid, acetic acid, formamide and pyrrole-2-carboxylic acid: an ab initio study*. Journal of Physical Chemistry A. 2005, Vol. 109, No. 29, s. 6397–6405.
  9. Góra R., Sokalski A., Leszczynski J., Pett V.B.: *The nature of interactions in the ionic crystal of 3-pentenenitrile, 2-nitro-5-oxo, ion(-1), sodium*. Journal of Physical Chemistry B. 2005, Vol. 109, No. 5, s. 2027–2033.
  10. Grabowski S.J., Sokalski A.: *Different types of hydrogen bonds: correlation analysis of interaction energy components*. Journal of Physical Organic Chemistry. 2005, Vol. 18, No. 8, s. 779–784.
  11. Grabowski S.J., Sokalski A., Leszczynski J.: *How short can the H...H intermolecular contact be?: New findings that reveal the covalent nature of extremely strong interactions*. Journal of Physical Chemistry A. 2005, Vol. 109, No. 19, s. 4331–4341.
  12. Hilpert K., Roszak S., Saloni J., Miller M., Lipkowski P., Leszczynski J.: *The dimerization of SnCl<sub>2(g)</sub>: mass spectrometric and theoretical studies*. Journal of Physical Chemistry A. 2005, Vol. 109, No. 7, s. 1286–1294.
  13. Janus K., Sworakowski J.: *Photochromizm of crown ethers with incorporated azobenzene moiety*. Journal of Physical Chemistry B. 2005, Vol. 109, No. 1, s. 93–101.
  14. Kishine J.I., Ohara T., Luty T., Yonemitsu K.: *Inter-chain Coulomb-lattice relaxation and multicriticality in charge transfer organic complexes*. Synthetic Metals. 2005, Vol. 154, No. 1–3, s. 257–260.
  15. Kluczyk A., Szeferczyk B., Amrhein N., Zoń J.: *(E)-Cinnamic acid analogues as inhibitors of phenylalanine ammonia-lyase and anthocyanin biosynthesis*. Polish Journal of Chemistry. 2005, Vol. 79, No. 3, s. 583–592.
  16. Lewanowicz A., Olszowski A., Dziekoński P., Leszczynski J.: *Spectroscopic characteristics of the micro-environmentally induced H-bond transformation in anil-type species: experimental and theoretical study*. Journal of Molecular Modeling. 2005, Vol. 11, No. 4/5, s. 398–406.
  17. Lutsyk P., Dzura L., Kutsenko A., Vertsimakha Y., Sworakowski J.: *Photovoltaic and optical properties of a polymer-PbS nanocomposite*. Semiconductor Physics, Quantum Electronics & Optoelectronics. 2005, Vol. 8, No. 3, s. 54–59.
  18. Michalkova A., Szymczak J.J., Leszczynski J.: *Adsorption of 2,4-dinitrotoluene on dickite: the role of H-bonding*. Structural Chemistry. 2005, Vol. 16, No. 3, s. 325–337.

19. Mirończuk A., Jankowski A., Chyla A., Ożyhar A., Dobryczycki P.: *The influence of ammonia, acetic acid and water vapour on the fluorescence of a 2-naphthol derivative in the Langmuir-Blodgett films*. Materials Science-Poland. 2005, Vol. 23, No. 1, s. 195–207.
20. Mora C., Latacz L., Nowak P.M., Rajkowski B., Dyonizy A.: *Effect of lumino-phores on silver halide emulsions*. Imaging Science Journal. 2005, Vol. 53, No. 4, s. 187–194.
21. Nešpůrek S., Wang G., Toman P., Sworakowski J., Bartkowiak W., Iwamoto M., Combellas C.: *Charge mobilities in molecular materials reversibly modified by light: towards a molecular switch*. Molecular Crystals and Liquid Crystals. 2005, Vol. 430, s. 127–133.
22. Niewodniczański W., Bartkowiak W., Leszczynski J.: *Reinvestigation of molecular structure and barrier to internal rotation of pyridinium N-phenolate betaine dye*. Journal of Molecular Modeling. 2005, Vol. 11, No. 4/5, s. 392–397.
23. Olszowski A., Lewanowicz A., Dziekoński P., Sokalski A., Leszczynski J.: *Environmentally induced H-bond transformation as a source of anil-type molecule specific solvatochromy*. Molecular Crystals and Liquid Crystals. 2005, Vol. 427, s. 245–258.
24. Ordon P., Komorowski L.: *DFT energy derivatives and their renormalization in molecular vibrations*. International Journal of Quantum Chemistry. 2005, Vol. 101, No. 6, s. 703–713.
25. Pawlik G., Mituś A., Miniewicz A., Sobolewska A.M., Kajzar F.: *Temperature dependence of the kinetics of diffraction gratings formation in a polymer matrix containing azobenzene chromophores: Monte Carlo simulations and experiment*. Molecular Crystals and Liquid Crystals. 2005, Vol. 426, s. 243–252.
26. Roszak S., Gee R.H., Balasubramanian K., Fried L.E.: *New theoretical insight into the interactions and properties of formic acid: development of a quantum-based pair potential for formic acid*. Journal of Chemical Physics. 2005, Vol. 123, No. 14, s. 144702(1–10).
27. Sheng Y., Roszak S., Szymczak J.J., Leszczynski J.: *Structures and energetics of extended proton-bound  $N_2H^{(+)}$ - $He_n$  ( $n = 1-17$ ) complexes*. Molecular Physics. 2005, Vol. 103, No. 6–8, s. 1091–1098.
28. Sidorowicz A., Mora C., Jabłonka S., Poła A., Modrzycka T., Mosiądz D., Michalak K.: *Spectral properties of two betaine-type cyanine dyes in surfactant micelles and in the presence of phospholipids*. Journal of Molecular Structure. 2005, Vol. 744–747, s. 711–716, 7.

29. Sinicropi A., Andruniów T., Ferre N., Basosi R., Olivucci M.: *Properties of the emitting state of the green fluorescent protein resolved at the CASPT2//CASSCF/CHARMM level*. Journal of the American Chemical Society. 2005, Vol. 127, No. 33, s. 11534–11535.
30. Skwara B., Góra R., Bartkowiak W.: *On the influence of non-additive interactions on the optical properties of the selected subsystems of crystalline urea*. Chemical Physics Letters. 2005, Vol. 406, No. 1–3, s. 29–37.
31. Strasburger K., Chojnacki H., Sokołowska A.: *Adiabatic potentials for the interaction of atomic antihydrogen with He and He<sup>(+)</sup>*. Journal of Physics B. 2005, Vol. 38, No. 17, s. 3091–3105.
32. Strasburger K.: *Born-Oppenheimer potential energy for interaction of antihydrogen with molecular hydrogen*. Journal of Physics B. 2005, Vol. 38, No. 17, s. 3197–3205.
33. Sworakowski J., Janus K., Nešpůrek S.: *Kinetics of photochromic reactions in condensed phases*. Advances in Colloid and Interface Science. 2005, Vol. 116, No. 1–3, s. 97–110.
34. Szymczak J.J., Roszak S., Skowroński P., Leszczynski J.: *The chemistry of lithium – modified carbonium*. Molecular Physics. 2005, Vol. 103, No. 15/16, s. 2215 – cations 2222.
35. Toman P., Bartkowiak W., Nešpůrek S., Sworakowski J., Zaleśny R.: *Quantum-chemical insight into the design of molecular optoelectrical switch*. Chemical Physics. 2005, Vol. 316, No. 1–3, s. 267–278.
36. Toman P., Nešpůrek S., Bartkowiak W., Sworakowski J.: *Excitations in oligosilanes with photochromic side groups*. Journal of Luminescence. 2005, Vol. 112, No. 1–4, s. 386–390.
37. Wang J., Roszak S., Gu J., Leszczynski J.: *Comprehensive global energy minimum modeling of the sarin-serine adduct*. Journal of Physical Chemistry B. 2005, Vol. 109, No. 2, s. 1006–1014.
38. Weiter M., Vala M., Salyk O., Zmeskal O., Nešpůrek S., Sworakowski J.: *Reversible formation of charge carrier traps in poly(phenylenevinylene) derivative due to the phototransformation of a photochromic additive*. Molecular Crystals and Liquid Crystals. 2005, Vol. 430, s. 227–233.
39. Wielgus P., Roszak S., Majumdar D., Leszczynski J.: *Thermodynamic properties of germanium/carbon microclusters*. Journal of Chemical Physics. 2005, Vol. 123, No. 23, s. 234309(1–8).

40. Zaleśny R., Bartkowiak W.: *Performance of the reduced-size polarized Z3PolX basis set in calculations of vibrational polarizabilities, infrared and Raman intensities: application to formaldehyde molecule*. International Journal of Quantum Chemistry. 2005, Vol. 104, No. 5, s. 660–666.

## 2004

1. Bartkiewicz S., Matczyszyn K., Myśliwiec J., Yaroshchuk O., Kosa T., Palffy-Muharey P.: *LC alignment controlled by photoordering and photorefraction in a command substrate*. Molecular Crystals and Liquid Crystals. 2004, Vol. 412, s. 301–312.
2. Bartkowiak W., Skwara B., Zaleśny R.: *The influence of solvent on the two-photon absorption cross section and hyperpolarizability of molecules exhibiting large solvatochromic shifts*. Journal of Computational Methods in Sciences and Engineering. 2004, Vol. 4, No. 4, s. 551–558.
3. Drożdżewski P., Kordon E., Roszak S.: *The studies of metal isotope and deuteration effects in vibrational spectra of palladium(II) complex with histamine*. International Journal of Quantum Chemistry. 2004, Vol. 96, No. 4, s. 355–364.
4. Dyguda-Kazimierowicz E.B., Szefczyk B., Sokalski A.: *The mechanism of phosphoryl transfer reaction and the role of active site residues on the basis of ribokinase-like kinases*. International Journal of Molecular Sciences. 2004, Vol. 5, Iss. 4, s. 141–153.
5. Gabryś B.J., Pesz K., Bartkiewicz S.: *Brownian motion, molecular motors and ratchets*. Physica. A, Statistical Mechanics and its Applications. 2004, Vol. 336, No. 1/2, s. 112–122.
6. Gee R.H., Roszak S., Balasubramanian K., Fried L.E.: *Ab initio based force field and molecular dynamics simulations of crystalline TATB*. Journal of Chemical Physics. 2004, Vol. 120, No. 15, s. 7059–7066.
7. Giju K.T., Roszak S., Góra R., Leszczynski J.: *The micro-solvation of  $\text{Na}^+$ : theoretical study of bonding characteristics in weakly bonded  $\text{Ar}_n\text{Na}^+$  ( $n = 1-8$ ) clusters*. Chemical Physics Letters. 2004, Vol. 391, [No. 1–3], s. 112–119.
8. Góra R., Bartkowiak W., Roszak S., Leszczynski J.: *Intermolecular interactions in solution: elucidating the influence of the solvent*. Journal of Chemical Physics. 2004, Vol. 120, No. 6, s. 2802–2813.
9. Gorb L., Podolyan Y., Dziekoński P., Sokalski A., Leszczynski J.: *Double-proton transfer in adenine-thymine and guanine-cytosine base pairs: A Post-Hartree-Fock ab initio study*. Journal of the American Chemical Society. 2004, Vol. 126, No. 32, s. 10119–10129.

10. Grabiec E., Schab-Balcerzak E., Sęk D., Sobolewska A.M., Miniewicz A.: *New polyamides with azo-chromophore groups*. Thin Solid Films. 2004, Vol. 453, No. 1, s. 367–371.
11. Grabowski S.J., Sokalski A., Leszczynski J.: *Is a  $\pi \dots H^+ \dots \pi$  complex hydrogen bonded?* Journal of Physical Chemistry A. 2004, Vol. 108, No. 10, s. 1806–1812.
12. Grabowski S.J., Sokalski A., Leszczynski J.: *Nature of  $X-H(+\delta) \dots (-\delta)H-Y$  dihydrogen bonds and  $X-H \dots \sigma$  interactions*. Journal of Physical Chemistry A. 2004, Vol. 108, No. 27, s. 5823–5830.
13. Grudniewski T., Parka J., Dąbrowski R., Stolarz Z., Miniewicz A.: *Photorefractive effects in pure multicomponent isothiocyanate liquid crystals under low power illumination*. Molecular Crystals and Liquid Crystals. 2004, Vol. 413, No. 1, s. 443–450.
14. Guerin L., Collet E., Lemee-Cailleau M.H., Buron-Le Cointe M., Cailleau H., Plech A., Wulff M., Koshihara S.Y., Luty T.: *Probing photoinduced phase transition in a charge-transfer molecular crystal by 100 picosecond X-ray diffraction*. Chemical Physics. 2004, Vol. 299, s. 163–170.
15. Hua X., van Deventer J.S.J., Roszak S., Leszczynski J.: *Ab initio study of dissolution reactions of five-membered aluminosilicate framework rings*. International Journal of Quantum Chemistry. 2004, Vol. 96, No. 4, s. 365–373.
16. Janus K., Sworakowski J.: *Analysis of first-order reactions with distributed parameters*. Structural Chemistry. 2004, Vol. 15, No. 5, s. 461–468.
17. Jonsell S., Froelich P., Eriksson S., Strasburger K.: *Strong nuclear force in cold antihydrogen-helium collisions*. Physical Review. A. 2004, Vol. 70, No. 6, s. 062708(1–6).
18. Kędzierski P., Wielgus P., Sikora A., Sokalski A., Leszczynski J.: *Visualization of the differential transition state stabilization within the active site environment*. International Journal of Molecular Sciences. 2004, Vol. 5, iss. 4, s. 186–195.
19. Kishine J., Luty T., Yonemitsu K.: *Ferroelectric phase transition, ionicity condensation, and multicriticality in charge-transfer organic complexes*. Physical Review. B. 2004, Vol. 69, s. 075115(1–5).
20. Komorowski L., Ordon P.: *Anharmonicity of a molecular oscillator*. International Journal of Quantum Chemistry. 2004, Vol. 99, No. 3, s. 153–160.
21. Lipiński J.: *Sum rules for nonlinear optical properties of molecules*. Chemical Physics Letters. 2004, Vol. 394, No. 4–6, s. 397–399.

22. Lipkowski P., Grabowski S.J., Robinson T.L., Leszczynski J.: *Properties of the C-H...H dihydrogen bond: an ab initio and topological analysis*. Journal of Physical Chemistry A. 2004, Vol. 108, No. 49, s. 10865–10872.
23. Luty T., Yonemitsu K.: *On thermo- and photo-induced symmetry-broken transformation in spin-crossover complex: cooperative activation*. Journal of the Physical Society of Japan. 2004, Vol. 73, No. 5, s. 1237–1243.
24. Miniewicz A., Michelotti F., Belardini A.: *Photoconducting polymer-liquid crystal structure studied by electroreflectance*. Journal of Applied Physics. 2004, Vol. 95, No. 3, s. 1141–1147.
25. Mirończyk A., Jankowski A., Chyla A., Ożyhar A., Dobryczycki P.: *Investigation of excited-state proton transfer in 2-naphthol derivatives included in Langmuir-Blodgett films*. Journal of Physical Chemistry A. 2004, Vol. 108, No. 25, s. 5308–5314.
26. Nešpůrek S., Sworakowski J., Combellas C., Wang G., Weiter M.: *A molecular device based on light controlled charge carrier mobility*. Applied Surface Science. 2004, Vol. 234, No. 1–4, s. 395–402.
27. Nowak P.M., Mora C., Rajkowski B., Latacz L., Dyonizy A.: *Sensitometric properties of silver halide light-sensitive emulsions obtained in presence of selected organic solvents*. Imaging Science Journal. 2004, Vol. 52, s. 35–40.
28. Pawlik G., Mituś A., Miniewicz A., Kajzar F.: *Monte Carlo simulations of temperature dependence of the kinetics of diffraction gratings formation in a polymer matrix containing azobenzene chromophores*. Journal of Nonlinear Optical Physics and Materials. 2004, Vol. 13, No. 3/4, s. 481–489.
29. Petsalakis I.D., Theodorakopoulos G., Góra R., Roszak S.: *Theoretical ab initio study on the electronic states of GaO and Ga<sub>2</sub>O*. Journal of Molecular Structure. Theochem. 2004, Vol. 672, No. 1–3, s. 105–111.
30. Ranaghan K.E., Ridder L., Szeferczyk B., Sokalski A., Hermann J.C., Mulholland A.J.: *Transition state stabilization and substrate strain in enzyme catalysis: ab initio QM/MM modelling of the chorismate mutase reaction*. Organic and Biomolecular Chemistry. 2004, Vol. 2, s. 968–980.
31. Rode M.F., Roszak S., Szymczak J.J., Sadlej J., Leszczynski J.: *The effect of electron detachment on the structure and properties of the chlorine-acetonitrile anionic complex*. Journal of Chemical Physics. 2004, Vol. 121, No. 13, s. 6277–6281.
32. Saloni J., Roszak S., Hilpert K., Miller M., Leszczynski J.: *Quantum chemical studies of neutral and ionized DyX, DyX<sub>2</sub>, and DyX<sub>3</sub> species (X = F, Cl, Br, I) and the implications for the mass spectra of gaseous DyX<sub>3</sub>*. European Journal of Inorganic Chemistry. 2004, Iss. 6, s. 1212–1218.

33. Saloni J., Roszak S., Miller M., Hilpert K., Leszczynski J.: *Sn<sub>2</sub>Br<sub>x</sub>I<sub>4</sub><sup>x</sup>(g) and Sn<sub>2</sub>Br<sub>y</sub>I<sub>3</sub><sup>y</sup> (x = 0–4, y = 0–3) species: mass spectrometric evidence and quantum-chemical studies*. Journal of Physical Chemistry A. 2004, Vol. 108, No. 13, s. 2418–2425.
34. Schab-Balcerzak E., Janeczek H., Kaczmarczyk B., Bednarski H., Sęk D., Miniewicz A.: *Epoxy resin cured with diamine bearing azobenzene group*. Polymer. 2004, Vol. 45, No. 8, s. 2483–2493.
35. Sheng Y., Roszak S., Leszczynski J.: *Microsolvation of N<sub>2</sub>H<sup>+</sup>: The nature of interactions in N<sub>2</sub>H(+)-(H<sub>2</sub>)<sub>n</sub> (n = 1–14) complexes*. Journal of Chemical Physics. 2004, Vol. 120, No. 9, s. 4324–4332.
36. Skwara B., Bartkowiak W., Leszczynski J.: *The influence of intermolecular interactions on second-order susceptibilities of molecular crystals: application to the m-nitroaniline crystal*. Structural Chemistry. 2004, Vol. 15, No. 5, s. 363–368.
37. Strasburger K.: *Dependence of the static leptonic properties on the internuclear distance in the H-H and He-H systems*. Journal of Physics. B. 2004, Vol. 37, No. 10, s. 2211–2219.
38. Strasburger K.: *Hydrogen-antihydrogen interaction: spectacular breakdown of the adiabatic approximation*. Journal of Physics. B. 2004, Vol. 37, No. 22, s. 4483–4492.
39. Strasburger K.: *Positronic formaldehyde – the configuration interaction study*. Structural Chemistry. 2004, Vol. 15, No. 5, s. 415–420.
40. Sworakowski J., Nešpůrek S., Toman P., Wang G., Bartkowiak W.: *Reversible mobility switching in molecular materials controlled by photochromic reactions*. Synthetic Metals. 2004, Vol. 147, No. 1–3, s. 241–246.
41. Szeftczyk B., Mulholland A.J., Ranaghan K.E., Sokalski A.: *Differential transition – state stabilization in enzyme catalysis: quantum chemical analysis of interactions in the chorismate mutase reaction and prediction of the optimal catalytic field*. Journal of the American Chemical Society. 2004, Vol. 126, No. 49, s. 16148–16159.
42. Szymczak J.J., Giju K.T., Roszak S., Leszczynski J.: *The Li<sup>+</sup> cation – the descendant of H<sup>+</sup> or an ancestor of Na<sup>+</sup>?: The properties of Li<sup>+</sup>Ar<sub>n</sub> (n = 1–6) clusters*. Journal of Physical Chemistry A. 2004, Vol. 108, No. 31, s. 6570–6574.
43. Szymczak J.J., Grabowski S.J., Roszak S., Leszczynski J.: *H...sigma interactions – an ab initio and „atoms in molecules” study*. Chemical Physics Letters. 2004, Vol. 393, No. 1–3, s. 81–86.

44. Taunamang H., Solyga M., Tija M.O., Miniewicz A.: *On the efficient mixed amplitude and phase grating recording in vacuum deposited Disperse Red 1*. Thin Solid Films. 2004, Vol. 461, No. 2, s. 316–324.
45. Turowska-Tyrk I., Grześniak K.: *Monitoring structural transformations in crystals: 7. 1-Chloroanthracene and its photodimer*. Acta Crystallographica. C. 2004, Vol. 60, pt. 2, s. 0146–0148.
46. Turowska-Tyrk I.: *Structural transformations in organic crystals during photochemical reactions*. Journal of Physical Organic Chemistry. 2004, Vol. 17, No. 10, s. 837–847.
47. Wójcik G., Mossakowska I.: *Thermal expansion studies of CaO.2Al<sub>2</sub>O<sub>3</sub>: A new refractory material*. Polish Journal of Chemistry. 2004, Vol. 78, No. 2, s. 273–278.
48. Zaleśny R., Sadlej A.J., Leszczynski J.: *Size-nonextensive contributions in singles-only CI*. Structural Chemistry. 2004, Vol. 15, No. 5, s. 379–384.
49. Zoń J., Szefczyk B., Sawka-Dobrowolska W., Gancarz R., Kucharska-Zoń M., Latajka R., Amrhein N., Miziak P., Szczepanik W.: *Experimental and ab initio calculated structures of 2-aminoindane-2-phosphonic acid, a potent inhibitor of phenylalanine ammonia-lyase, and theoretical studies of its binding to the model enzyme structure*. New Journal of Chemistry. 2004, Vol. 28, No. 8, s. 1048–1055.
50. Żurek J., Bowman A.L., Sokalski A., Mulholland A.: *MM and QM/MM modeling of threonyl-tRNA synthetase: model testing and simulations*. Structural Chemistry. 2004, Vol. 15, No. 5, s. 405–414.

## 2003

1. Bartkowiak W., Zaleśny R., Leszczynski J.: *Relation between bond-length alternation and two-photon absorption of a push-pull conjugated molecules: a quantum-chemical study*. Chemical Physics. 2003, Vol. 287, No. 1/2, s. 103–112.
2. Basak S.C., Balasubramanian K., Gute B.D., Mills D., Gorczynska A., Roszak S.: *Prediction of cellular toxicity of halocarbons from computed chemodescriptors: a hierarchical QSAR approach*. Journal of Chemical Information and Computer Sciences. 2003, Vol. 43, s. 1103–1109.
3. Chojnacki H.: *Quantum chemical studies on newly synthesized tin anticancer compounds*. Journal of Molecular Structure. Theochem. 2003, Vol. 630, No. 1–3, s. 291–295.

4. Chojnacki H.: *Special issue on proton transfer processes*. International Journal of Molecular Sciences. 2003, Vol. 4, iss. 7, s. 408–409.
5. Chojnacki H.: *Studies on electronic charge of the hydrogen bond proton in model molecular system*. International Journal of Molecular Sciences. 2003, Vol. 4, Iss. 7, s. 481–485.
6. Collet E., Lemee-Cailleau M.H., Buron-Le Cointe M., Cailleau H., Wulff M., Luty T., Koshihara S.Y., Meyer M., Toupet L., Rabiller P., Techert S.: *Laser-induced ferroelectric structural order in an organic charge-transfer crystal*. Science. 2003, Vol. 300, s. 612–615.
7. Dziekoński P., Sokalski A., Podolyan Y., Leszczynski J.: *Nonempirical analysis of the catalytic activity of the molecular environment – optimal static and dynamic catalytic fields for double proton transfer in formamide-formamidine complex*. Chemical Physics Letters. 2003, Vol. 367, No. 3/4, s. 367–375.
8. Fabiański R., Kuchta B.: *Polymorphism of cyanoadamantane crystal*. Phase Transitions. 2003, Vol. 76, No. 9/10, s. 815–821.
9. Flinn C., Poirier R.A., Sokalski A.: *Ab initio study of the deamination of formamidine*. Journal of Physical Chemistry A. 2003, Vol. 107, No. 50, s. 11174–11181.
10. Hill G., Forde G., Hill N., Lester W.A. Jr, Sokalski A., Leszczynski J.: *Interaction energies in stacked DNA bases?: How important are electrostatics?*. Chemical Physics Letters. 2003, Vol. 381, No. 5/6, s. 729–732.
11. Kędzierski P., Sokalski A., Cheng H., Mitchell J., Leszczynski J.: *DFT study of the reaction proceeding in the cytidine deaminase*. Chemical Physics Letters. 2003, Vol. 381, No. 5/6, s. 660–665.
12. Komorowski L., Ordon P.: *DFT analysis of fluctuations of electronegativity and hardness of a molecular oscillator*. International Journal of Quantum Chemistry. 2003, Vol. 91, No. 3, s. 398–403.
13. Komorowski L., Ordon P.: *Fluctuations in electronegativity and global hardness induced by the molecular vibrations*. Journal of Molecular Structure. Theochem. 2003, Vol. 630, No. 1–3, s. 25–32.
14. Lipkowski P., Koll A., Karpfen A., Wolschann P.: *Steric enhancement of the strength of intramolecular hydrogen bond in 3-Cl substituted 2-(N-dimethylaminomethyl) phenols*. Chemical Physics Letters. 2003, Vol. 370, No. 1/2, s. 74–82.
15. Luty T.: *Thermo- and photo-induced multistabilities: solid state reaction and polymorphism*. Phase Transitions. 2003, Vol. 76, No. 9/10, s. 857–865.

16. Majumdar D., Roszak S., Balasubramanian K., Nitsche H.: *Theoretical study of aqueous uranyl carbonate ( $UO_2CO_3$ ) and its hydrated complexes:  $UO_2CO_3 \cdot nH_2O$  ( $n = 1-3$ )*. Chemical Physics Letters. 2003, Vol. 372, No. 1/2, s. 232–241.
17. Majumdar D., Roszak S., Balasubramanian K.: *Electronic structure and spectroscopic properties of electronic states of  $VC_2$ ,  $VC_2^-$ , and  $VC_2^+$* . Journal of Chemical Physics. 2003, Vol. 118, No. 1, s. 130–141.
18. Matczyszyn K., Sworakowski J.: *Phase change in azobenzene derivative-doped liquid crystal controlled by the photochromic reaction of the dye*. Journal of Physical Chemistry B. 2003, Vol. 107, No. 25, s. 6039–6045.
19. Miniewicz A., Gniewek A., Parka.: *Liquid crystals for photonic applications*. Optical Materials (Amsterdam). 2003, Vol. 21, No. 1–3, s. 605–610.
20. Nešpůrek S., Sworakowski J., Kadashchuk A., Toman P.: *Polysilylenes: charge carrier transport and photogeneration*. Journal of Organometallic Chemistry. 2003, Vol. 685, No. 1/2, s. 269–279.
21. Pawlik G., Mituś A., Miniewicz A., Kajzar F.: *Kinetics of diffraction gratings formation in a polymer matrix containing azobenzene chromophores: experiments and Monte Carlo simulations*. Journal of Chemical Physics. 2003, Vol. 119, No. 13, s. 6789–6801.
22. Ranaghan K.E., Ridder L., Szeferczyk B., Sokalski A., Hermann J.C., Mulholland A.J.: *Insights into enzyme catalysis from QM/MM modelling: transition state stabilization in chorismate mutase*. Molecular Physics. 2003, Vol. 101, No. 17, s. 2695–2714.
23. Roszak S., Gee R.H., Balasubramanian K., Fried L.E.: *Molecular interactions of TATB clusters*. Chemical Physics Letters. 2003, Vol. 374, No. 3/4, s. 286–296.
24. Roszak S., Leszczynski J.: *Ab initio studies of the microsolvation of ions*. Journal of Physical Chemistry A. 2003, Vol. 107, No. 7, s. 949–955.
25. Schab-Balcerzak E., Grabiec E., Sęk D., Miniewicz A.: *New azobenzene chromophores as monomers for synthesis of polyesters*. Polymer Journal. 2003, Vol. 35, No. 11, s. 851–858.
26. Sęk D., Grabiec E., Miniewicz A.: *Investigations of polymers with chromophore: Units I. Synthesis and properties of new poly(ester-imide)s from 2,4-dihydroxy-4'-nitroazobenzene*. Polymer Journal. 2003, Vol. 35, No. 10, s. 749–756.
27. Skarżewski J., Zielińska-Błajet M., Roszak S., Turowska-Tyrk I.: *Cyclization of 1,3-diaryl-3-phenylsulfanyl-1-propanols to thiochromas with the participation of [1,3]-PhS shift*. Tetrahedron. 2003, Vol. 59, No. 20, s. 3621–3626.

28. Sołoducho J., Doskocz J., Cabaj J., Roszak S.: *Practical synthesis of bis-substituted tetrazines with two pendant 2-pyrrolyl or 2-thienyl groups, precursors of new conjugated polymers*. Tetrahedron. 2003, Vol. 59, No. 26, s. 4761–4766.
29. Sworakowski J., Ułański J.: *Electrical properties of organic materials*. Annual Reports on the Progress of Chemistry. C, Physical Chemistry. 2003, Vol. 99, s. 87–125.
30. Szymczak J., Roszak S., Góra R., Leszczynski J.: *Molecular properties of protonated homogeneous and mixed carbon oxide and carbon dioxide clusters*. Journal of Chemical Physics. 2003, Vol. 119, No. 13, s. 6560–6570.
31. Turowska-Tyrk I., Grześniak K., Trzop E., Zych T.: *Monitoring structural transformations in crystals: Pt. 4. Monitoring structural changes in crystals of pyridine analogs of chalcone during [2 + 2]-photodimerization and possibilities of the reaction in hydroxy derivatives*. Journal of Solid State Chemistry. 2003, Vol. 174, No. 2, s. 459–465.
32. Turowska-Tyrk I., Trzop E.: *Monitoring structural transformations in crystals: [Pt.] 6. The [4 + 4] photodimerization of 9-methylanthracene*. Acta Crystallographica. B. 2003, Vol. 59, pt. 6, s. 779–786.
33. Turowska-Tyrk I.: *Monitoring initial structural changes in a crystal during photo-induced disappearance of its diffracting properties*. Chemical Physics. 2003, Vol. 288, No. 2/3, s. 241–247.
34. Turowska-Tyrk I.: *Monitoring structural transformations in crystals: [Pt.] 5. A topotactic [2+2]-photodimerization reaction*. Acta Crystallographica. B. 2003, Vol. 59, pt. 5, s. 670–675.
35. Zaleśny R., Bartkowiak W., Champagne B.: *Ab initio calculations of doubly resonant sum-frequency generation second-order polarizabilities of LiH*. Chemical Physics Letters. 2003, Vol. 380, No. 5/6, s. 549–555.
36. Zaleśny R., Bartkowiak W., Leszczynski J.: *Theoretical study of the two-photon absorption in photochromic fulgides*. Journal of Luminescence. 2003, Vol. 105, No. 2–4, s. 111–116.
37. Zhivkov I., Danev G., Wang G., Nešpůrek S., Sworakowski J.: *Charge injection into poly[methyl(phenyl)silylene]*. Journal of Materials Science. Materials in Electronics. 2003, Vol. 14, No. 10–12, s. 829–830.

## 2002

1. Bartkiewicz S., Matczyszyn K., Myśliwiec J., Miniewicz A., Sahraoui B., Martineau C., Blanchard P., Frere P., Roncali J., Kajzar F.: *Liquid crystal panel with dye doped*

- PVK layer for real time holography processes*. Molecular Crystals and Liquid Crystals Science and Technology. A. 2002, Vol. 374, s. 85–90.
2. Bartkiewicz S., Miniewicz A., Sahraoui B., Kajzar F.: *Dynamic charge-carrier-mobility-mediated holography in thin layers of photoconducting polymers*. Applied Physics Letters. 2002, Vol. 81, No. 20, s. 3705–3707.
  3. Bartkowiak W., Zalesny R., Kowal M., Leszczynski J.: *The influence of the solute/solvent interactions on the first-order hyperpolarizability in urea molecule: A quantum chemical study*. Chemical Physics Letters. 2002, Vol. 362, No. 3/4, s. 224–228.
  4. Borzechowska M., Trush V., Turowska-Tyrk I., Amirkhanov W., Legendziewicz J.: *Spectroscopic and magnetic studies of mixed lanthanide complexes: LnL<sub>3</sub>alfa,alfa'Dipy in solution and in solid*. Journal of Alloys and Compounds. 2002, Vol. 341, No. 1/2, s. 98–106.
  5. Chojnacki H.: *Quantum chemical studies on the double proton transfer in benzoic and o-chlorobenzoic acid dimers*. Polish Journal of Chemistry. 2002, Vol. 76, No. 2/3, s. 295–300.
  6. Collet E., Lemee-Cailleau M.H., Buron-Le Cointe M., Cailleau H., Ravy S., Luty T., Berar J.F., Czarnecki P., Karl N.: *Direct evidence of lattice-relaxed charge transfer exciton strings*. Europhysics Letters. 2002, Vol. 57, No. 1, s. 67–73.
  7. Dubis A.T., Grabowski S.J., Romanowska D.B., Misiaszek T., Leszczynski J.: *Pyrrole-2-carboxylic acid and its dimers: molecular structures and vibrational spectrum*. Journal of Physical Chemistry A. 2002, Vol. 106, No. 44, s. 10613–10621.
  8. Dyonizy A., Nowak P.M.: *Electron microscopic analysis of the structure of the silver halide light-sensitive layers*. Optica Applicata. 2002, Vol. 32, No. 1/2, s. 93–101.
  9. Dziekoński P., Sokalski A., Szyja B., Leszczynski J.: *Physical nature of catalytic effects of Si → Al substitutions in ZMS-5 zeolite for propylene protonation reaction*. Chemical Physics Letters. 2002, Vol. 364, No. 1/2, s. 133–138.
  10. Fabiański R., Firlej L., Kuchta B.: *Computer modeling of disordered molecular solids: six-state model of glassy crystal cyanoadamantane*. Journal of Chemical Physics. 2002, Vol. 116, No. 23, s. 10356–10360.
  11. Fabiański R., Firlej L., Kuchta B.: *Six-state model of cyanoadamantane crystal: MC simulations*. Computer Physics Communications. 2002, Vol. 147, s. 174–177.
  12. Fabiański R., Firlej L., Zahab A., Kuchta B.: *Relationships between crystallinity, oxygen diffusion and electrical conductivity of evaporated C<sub>70</sub> thin films*. Solid State Sciences. 2002, Vol. 4, s. 1009–1015.

13. Giju K.T., Roszak S., Leszczynski J.: *A theoretical study of protonated argon clusters:  $Ar_nH^+$  ( $n = 1-7$ )*. Journal of Chemical Physics. 2002, Vol. 117, No. 10, s. 4803–4809.
14. Góra R., Bartkowiak W., Roszak S., Leszczynski J.: *A new theoretical insight into the nature of intermolecular interactions in the molecular crystal of urea*. Journal of Chemical Physics. 2002, Vol. 117, No. 3, s. 1031–1039.
15. Grudniewski T., Parka J., Dąbrowski R., Januszko A., Miniewicz A.: *Investigations of the diffraction efficiency in dye-doped LC cells under low frequency AC voltage*. Opto-Electronics Review. 2002, Vol. 10, No. 1, s. 11–15.
16. Huskowska E., Turowska-Tyrk I., Legendziewicz J., Riehl J.P.: *The structure and spectroscopy of lanthanide(III) complexes with 2,2'-bipyridine-1,1'-dioxide in solution and in the solid state: effects of ionic size and solvent on photophysics, ligand structure and coordination*. New Journal of Chemistry. 2002, Vol. 26, No. 10, s. 1461–1467.
17. Janus K., Koshets I.A., Sworakowski J., Nešpůrek S.: *An approximate non-isothermal method to study kinetic processes controlled by a distribution of rate constants: the case of a photochromic azobenzene derivative dissolved in a polymer matrix*. Journal of Materials Chemistry. 2002, Vol. 12, No. 6, s. 1657–1663.
18. Janus K., Sworakowski J., Luboch E.: *Kinetics of photochromic reactions in a 10-membered dibenzoazo crown ether*. Chemical Physics. 2002, Vol. 285, No. 1, s. 47–54.
19. Kapała J., Roszak S., Nunziante-Cesaro S., Miller M.: *Vaporization of  $LnCl_3$  and thermochemistry of  $Ln_2Cl_6(g)$ ,  $Ln = Ce, Pr, Nd, Dy$* . Journal of Alloys and Compounds. 2002, Vol. 345, No. 1/2, s. 90–99.
20. Kaplan I.G., Murrell J.N., Roszak S., Leszczynski J.: *Ab initio model potentials for the alkaline-earth trimers  $Be_3$ ,  $Mg_3$ , and  $Ca_3$* . Molecular Physics. 2002, Vol. 100, No. 6, s. 843–849.
21. Komorowska K., Miniewicz A., Parka J., Kajzar F.: *Self-induced nonlinear Zernike filter realized with optically addressed liquid crystal spatial light modulator*. Journal of Applied Physics. 2002, Vol. 92, No. 10, s. 5635–5641.
22. Lipiński J.: *On the consequences of the violation of the Hellmann-Feynman theorem in calculations of electric properties of molecules*. Chemical Physics Letters. 2002, Vol. 363, No. 3/4, s. 313–318.
23. Lorenc J., Kucharska E., Michalski J., Hanuza J., Mugeński E., Chojnacki H.: *Excited electronic states of 2-ethylamino-(3 or 5-methyl)-4-nitropyridine*. Journal of Molecular Structure. 2002, Vol. 614, No. 1–3, s. 257–266.

24. Luty T., Cailleau H., Koshihara S.Y., Collet E., Takesada M., Lemee-Cailleau M.H., Buron-Le Cointe M., Nagaosa N., Tokura Y., Zienkiewicz E., Ouladdiaf B. *Static and dynamic order of cooperative multi-electron transfer*. Europhysics Letters. 2002, Vol. 59, No. 4, s. 619–625.
25. Luty T., Ogawa T., Okajima Y., Zienkiewicz E., Cailleau H., Collet E., Koshihara S.Y., Lemee-Cailleau M.H., Buron M.: *Photo-induced transformations: three states model*. Phase Transitions. 2002, Vol. 75, No. 7/8, s. 659–671.
26. Luty T., Ordon P., Eckhardt C.J.: *A model for mechanochemical transformations: applications to molecular hardness, instabilities, and shock initiation of reaction*. Journal of Chemical Physics. 2002, Vol. 117, No. 4, s. 1775–1785.
27. Matczyszyn K., Bartkiewicz S., Sahraoui B.: *A new holographic system: liquid crystal doped with photochromic molecules*. Optical Materials (Amsterdam). 2002, Vol. 20, No. 1, s. 57–61.
28. Miniewicz A., Komorowska K., Sęk D., Schab-Balcerzak E., Solyga M.: *Photoinduced optical anisotropy in azo-dye doped polyimide films*. Polish Journal of Chemistry. 2002, Vol. 76, No. 2/3, s. 395–407.
29. Myśliwiec J., Miniewicz A., Bartkiewicz S.: *Influence of light on self-diffraction process in liquid crystal cells with photoconducting polymeric layers*. Opto-Electronics Review. 2002, Vol. 10, No. 1, s. 53–58.
30. Nowak P.M., Rajkowski B.: *Review of empirical models of photographic recording of image information*. Optica Applicata. 2002, Vol. 32, No. 1/2, s. 103–112.
31. Palewska K., Chojnacki H.: *A possible mechanism of reversible photocyclization of [5]-helicene in Shpol'skii-type matrices at 4.2 K*. Journal of Molecular Structure. 2002, Vol. 611, No. 1–3, s. 23–32.
32. Palewska K., Lipiński J., Misiaszek T., Sworakowski J.: *Effect of solute-solvent compatibility on total luminescence spectra of perylene in Shpol'skii matrixes at liquid helium temperature*. Journal of Physical Chemistry A. 2002, Vol. 106, s. 4552–4557.
33. Pesz K., Gabryś B.J., Bartkiewicz S.: *Analytical solution for the Feynman ratchet*. Physical Review E. 2002, Vol. 66, No. 6, s. 061103(1–7).
34. Pesz K.: *A class of Fokker-Planck equations with logarithmic factors in diffusion and drift terms*. Journal of Physics A. 2002, Vol. 35, No. 8, s. 1827–1832.
35. Pruchnik F.P., Bańbuła M., Ciunik Z., Chojnacki H., Latocha M., Skop B., Wilczok T., Opolski A., Wietrzyk J., Nasulewicz A.: *Structure, properties and*

- cytostatic activity of triorganotin (aminoaryl)carboxylates*. European Journal of Inorganic Chemistry. 2002, No. 12, s. 3214–3221.
36. Pruchnik F.P., Bańbuła M., Ciunik Z., Chojnacki H., Skop B., Latocha M., Wilczok T.: *Structure, properties and in vitro cytotoxic activity of hexakis(2-cyanoethyl)ditin(III)*. Journal of Inorganic Biochemistry. 2002, Vol. 90, No. 3/4, s. 149–154.
37. Pruchnik F., Bańbuła M., Ciunik Z., Chojnacki H., Latocha M., Skop B., Wilczok T.: *Di-n-butyltin aminoarylcarboxylates: structure, properties and in vitro antitumor activity*. Applied Organometallic Chemistry. 2002, Vol. 16, No. 10, s. 587–592.
38. Rajkowski B., Latacz L.: *Model examination of the influence of edge effects on the acutance of photographic image*. Optica Applicata. 2002, Vol. 32, No. 1/2, s. 121–127.
39. Rajkowski B.: *Influence of the rate of photographic development process on the edge effects*. Optica Applicata. 2002, Vol. 32, No. 1/2, s. 113–119.
40. Roszak S., Majumdar D., Balasubramanian K.: *Electronic structure and spectroscopic properties of electronic states of  $ScC_3$  and  $ScC_3^-$* . Journal of Chemical Physics. 2002, Vol. 116, No. 23, s. 10238–10246.
41. Sahraoui B., Fuks-Janczarek I., Bartkiewicz S., Matczyszyn K., Myśliwiec J., Kityk I.V., Berdowski J., Allard E., Cousseau J.: *Enhancement of third-order optical susceptibility of  $C_{60}$ -TTF compounds using nematic liquid crystal*. Chemical Physics Letters. 2002, Vol. 365, No. 3/4, s. 327–332.
42. Sheng Y., Góra R., Roszak S., Kaczorowska M., Leszczynski J.: *The molecular structures, energetics, and nature of interactions in  $Ar_n^-N_2H^+$  ( $n = 1-12$ ) complexes*. Journal of Physical Chemistry A. 2002, Vol. 106, No. 46, s. 11162–11167.
43. Skarżewski J., Wojaczyńska E., Turowska-Tyrk I.: *Sequential asymmetric dihydroxylation and sulfoxidation of homoallylic sulfides: Stereochemical aspects of the preparation of new trifunctional chiral building blocks*. Tetrahedron: Asymmetry. 2002, Vol. 13, No. 4, s. 369–375.
44. Śliwińska E., Palewska K., Lewanowicz A., Lipiński J., Sworakowski J., Gancarz R., Nešpůrek S.: *Spectroscopic studies of two dynamically different 1,4-dihydropyridine structures*. Polish Journal of Chemistry. 2002, Vol. 76, No. 2/3, s. 235–247.
45. Śliwińska E., Sworakowski J., Ihmels H.: *Differential scanning calorimetry in studies of solid-state reactions in photochromic materials*. Journal of Photochemistry and Photobiology A. 2002, Vol. 151, No. 1–3, s. 83–88.

46. Strasburger K., Chojnacki H.: *Helium-antihydrogen interaction: the Born-Oppenheimer potential energy curve*. Physical Review Letters. 2002, Vol. 88, No. 16, s. 163201(1–4).
47. Strasburger K.: *Accurate Born-Oppenheimer potential energy curve for the hydrogen-antihydrogen system*. Journal of Physics. B. 2002, Vol. 35, No. 19, s. L435–L440.
48. Szefczyk B., Sokalski A., Leszczynski J.: *Optimal methods for calculation of the amount of intermolecular electron transfer*. Journal of Chemical Physics. 2002, Vol. 117, No. 15, s. 6952–6958.
49. Szostak M.M., Czarnecki M.: *Thermal and Near-IR photochemical generation of polarons in m-nitroaniline crystals. Application of 2D correlation FT-NIR spectroscopy*. Polish Journal of Chemistry. 2002, Vol. 76, No. 2/3, s. 419–433.
50. Tsaryuk V., Turowska-Tyrk I., Legendziewicz J., Zolin V., Szostak R., Puntus L.: *Spectra and details of the structure of europium aliphatic carboxylates with 1,10-phenanthroline derivatives*. Journal of Alloys and Compounds. 2002, Vol. 341, s. 323–332.
51. Turowska-Tyrk I.: *Monitoring cooperative effects in crystal of 2-benzyl-5-benzylidenecyclopentanone*. Chemical Physics Letters. 2002, Vol. 361, No. 1/2, s. 115–120.
52. Wójcik G., Holband J.: *Variable-temperature studies of the 4-isopropylphenol crystal structure from X-ray diffraction: Comparison of thermal expansion and molecular dynamics with spectroscopic results*. Acta Crystallographica. B. 2002, Vol. 58, pt. 4, s. 684–689.
53. Wójcik G., Mossakowska I., Holband J., Bartkowiak W.: *Atomic thermal motions studied by variable-temperature X-ray diffraction and related to non-linear optical properties of crystalline meta-dinitrobenzene*. Acta Crystallographica B. 2002, Vol. 58, pt. 6, s. 998–1004.
54. Zaleśny R., Bartkowiak W., Styrcz S., Leszczynski J.: *Solvent effects on conformationally induced enhancement of the two-photon absorption cross section of a pyridinium-N-phenolate betaine dye: A quantum chemical study*. Journal of Physical Chemistry A. 2002, Vol. 106, No. 16, s. 4032–4037.
55. Zawisza I., Bilewicz R., Janus K., Sworakowski J., Luboch E., Biernat J.F.: *Comparison of Z $\leftrightarrow$ E isomerization in Langmuir-Blodgett layers and in solution*. Materials Science & Engineering C. 2002, Vol. 22, No. 1, s. 91–98.

56. Zilberberg I., Góra R., Zhidomirov G.M., Leszczynski J.: *Bonding in the oxo ferrous iron species: a complete active-space selfconsistent-field theory verification of the molecular-oxygen-like pattern*. Journal of Chemical Physics. 2002, Vol. 117, No. 15, s. 7153–7161.

## 2001

1. Balawender R., De Proft F., Geerlings P.: *Nuclear Fukui function and Berlin's binding function: Prediction of the Jahn–Teller distortion*. Journal of Chemical Physics. 2001, Vol. 114, No. 10, s. 4441–4449.
2. Balawender R., Geerlings P.: *Nuclear Fukui function from coupled perturbed Hartree-Fock equations*. Journal of Chemical Physics. 2001, Vol. 114, No. 2, s. 682–691.
3. Balawender R., Safi B., Geerlings P.: *Solvent effect on the global and atomic DFT-based reactivity descriptors using the effective fragment potential model*. Journal of Physical Chemistry A. 2001, Vol. 105, No. 27, s. 6703–6710.
4. Bartkiewicz S., Matczyszyn K., Miniewicz A., Kajzar F.: *High gain of light in photoconducting polymer – nematic liquid crystal hybrid structures*. Optics Communications. 2001, Vol. 187, No. 1–3, s. 257–261.
5. Bartkowiak W., Strasburger K., Leszczynski J.: *Studies of molecular hyperpolarizabilities (beta, gamma) for 4-nitroaniline (PNA): The application of quantum mechanical/Langevin dipoles/Monte Carlo (QM/LD/MC) and sum-over-orbitals (SOO) methods*. Journal of Molecular Structure. Theochem. 2001, Vol. 549, No. 1/2, s. 159–163.
6. Bartkowiak W., Zaleśny R., Niewodniczański W., Leszczynski J.: *Quantum chemical calculations of the first- and second-order hyperpolarizabilities of molecules in solutions*. Journal of Physical Chemistry A. 2001, Vol. 105, No. 47, s. 10702–10710.
7. Chojnacki H., Kołodziejczyk W., Pruchnik F.: *Quantum chemical studies on molecular and electronic structure of platinum and tin adducts with guanine*. International Journal of Molecular Sciences. 2001, Vol. 2, s. 148–155.
8. Chyla A., Lewandowska A., Sołoducho J., Górecka-Drzazga A., Szablewski M.: *4-t-butyl-CuPc-PODT molecular composite material for an effective gas sensor*. IEEE Transactions on Dielectrics and Electrical Insulation. 2001, Vol. 8, No. 3, s. 559–565.

9. Dziekoński P., Sokalski A., Leszczynski J.: *Physical nature of environmental effects on intermolecular proton transfer in  $(O_2NOH...NH_3)(H_2O)_n$  and  $(ClH...NH_3)(H_2O)_n$  ( $n = 1-3$ ) complexes*. Chemical Physics. 2001, Vol. 272, No. 1, s. 37–45.
10. Góra R., Roszak S., Leszczynski J.: *The molecular structures and nature of interactions in  $CH_3^+Ar_n$  ( $n = 1-8$ ) complexes*. Journal of Chemical Physics. 2001, Vol. 115, No. 2, s. 771–777.
11. Grembecka J., Sokalski A., Kafarski P.: *Quantum chemical analysis of the interactions of transition state analogs with leucine aminopeptidase*. International Journal of Quantum Chemistry. 2001, Vol. 84, No. 2, s. 302–310.
12. Hill G., Góra R., Roszak S., Leszczynski J.: *The structures and properties of cis- and trans- $MeCl_2(NH_3)_2$ ,  $Me = Pd$  and  $Pt$  complexes, in ground and excited states*. International Journal of Quantum Chemistry. 2001, Vol. 83, No. 3/4, s. 213–219.
13. Holband J., Jurkin M., Wójcik G., Holband T: *2-(5-Chloropyridin-2-yl)-2,3-dihydro-1H-isoindole-1,3-dione*. Acta Crystallographica E. 2001, Vol. 57, pt. 3, s. 250–251.
14. Holband J., Wójcik G., Ziara Z., Kafarski P.: *Conformational polymorphism of diethyl 1-(phthalylglycyloxy)-2-phthalylaminoethenephosphonate*. Journal of Molecular Structure. 2001, Vol. 595, No. 1–3, s. 167–174.
15. Kaczorowska M., Roszak S., Leszczynski J.: *Are the properties of shells ligand dependent? An ab initio study of mixed  $H_3^+Ar_n(H_2)_m$  ( $n + m = 6$ ) cations*. Journal of Physical Chemistry A. 2001, Vol. 105, No. 33, s. 7938–7944.
16. Kaplan I.G., Roszak S., Leszczynski J.: *Binding in clusters with closed-subshell atoms (alkaline-earth elements)*. Advances in Quantum Chemistry. 2001, Vol. 40, s. 257–278.
17. Kędzierski P., Moreton K., Clarke A.R., Holbrook J.J.: *The A245K mutation exposes another stage of the bacterial L-lactate dehydrogenase reaction mechanism*. Biochemistry. 2001, Vol. 40, No. 24, s. 7247–7252.
18. Kędzierski P., Sokalski A.: *Analysis of the transferability of atomic multipoles for amino acids in modeling macromolecular charge distribution from fragments*. Journal of Computational Chemistry. 2001, Vol. 22, No. 10, s. 1082–1097.
19. Komorowska K., Pawlik G., Mituś A., Miniewicz A.: *Electro-optic phenomena in nematic liquid crystals studied experimentally and by Monte-Carlo simulations*. Journal of Applied Physics. 2001, Vol. 90, No. 4, s. 1836–1842.
20. Komorowski L., Ordon P.: *Vibrational softening of diatomic molecules*. Theoretical Chemistry Accounts. 2001, Vol. 105, No. 4/5, s. 338–344.

21. Kowal M., Góra R., Roszak S., Leszczynski J.: *H<sub>2</sub>O and its neutral precursors: similarities and differences*. Journal of Chemical Physics. 2001, Vol. 115, No. 20, s. 9260–9265.
22. Kowal M., Roszak S., Leszczynski J.: *The influence of the molecular charge on potential energy curves for the proton transfer in electronic ground and excited states*. Journal of Chemical Physics. 2001, Vol. 114, No. 19, s. 8251–8256.
23. Latacz L., Nowak P.M.: *Model examination of application of fluorescent substance to silver halide light-sensitive layers*. Optica Applicata. 2001, Vol. 31, No. 1, s. 165–175.
24. Latacz L., Nowak P.M.: *Model examination of the crossover effect in two-layer light-sensitive system*. Optica Applicata. 2001, Vol. 31, No. 1, s. 177–184.
25. Latacz L., Nowak P.M.: *Model examination of the reflex-halation in single-layer light-sensitive system*. Optica Applicata. 2001, Vol. 31, No. 2, s. 499–506.
26. Leontidis E., Heinz H., Palewska K., Wallenborn E.-U., Suter U.W.: *Normal and defective perylene substitution sites in alkane crystals*. Journal of Chemical Physics. 2001, Vol. 114, No. 7, s. 3224–3235.
27. Luty T.: *Lattice mediation in thermo- and photo-induced reactions; co-operative activation*. Molecular Crystals and Liquid Crystals. 2001, Vol. 356, s. 539–548.
28. Majumdar D., Roszak S., Balasubramanian K.: *Interaction of benzene (Bz) with Pt and Pt<sub>2</sub>: a theoretical study on Bz-Pt<sub>2</sub>, Bz<sub>2</sub>-Pt, Bz<sub>2</sub>-Pt<sub>2</sub>, and Bz<sub>3</sub>-Pt<sub>2</sub> clusters*. Journal of Chemical Physics. 2001, Vol. 114, No. 23, s. 10300–10310.
29. Matczyszyn K., Bartkowiak W., Leszczynski J.: *Influence of the environment on kinetics and electronic structure of asymmetric azobenzene derivatives – experiment and quantum-chemical calculations*. Journal of Molecular Structure. 2001, Vol. 565/566, s. 53–57.
30. Miniewicz A., Komorowska K., Vanhanen J., Parka J.: *Surface-assisted optical storage in a nematic liquid crystal cell via photoinduced charge-density modulation*. Organic Electronics. 2001, Vol. 2, No. 3/4, s. 155–163.
31. Nešpůrek S., Pflieger J., Brynda E., Kminek I., Kadashchuk A., Vakhnin A., Sworakowski J.: *Poly(silylene)s: effect of polar acceptor side groups on the charge carrier photogeneration and transport*. Molecular Crystals and Liquid Crystals Science and Technology A. 2001, Vol. 355, s. 191–216.
32. Nešpůrek S., Sworakowski J., Kadashchuk A.: *The influence of dipolar species on charge carrier transport in a linear polysilicon*. IEEE Transactions on Dielectrics and Electrical Insulation. 2001, Vol. 8, No. 3, s. 432–441.

33. Rajkowski B., Nowak P.M.: *Model examinations of edge effects in light-sensitive materials*. *Optica Applicata*. 2001, Vol. 31, No. 1, s. 185–191.
34. Rajkowski B., Nowak P.M.: *Modelling of edge effects taking account of the diffusion phenomenon*. *Optica Applicata*. 2001, Vol. 31, No. 2, s. 489–497.
35. Roszak S., Koski W.S., Kaufman J.J., Balasubramanian K.: *Structures and electron attachment properties of halomethanes ( $CX_nY_m$ ,  $X = H, F$   $Y = Cl, Br$ ,  $I$   $n = 0, 4$ ;  $m = 4 - n$ )*. *SAR and QSAR in Environmental Research*. 2001, Vol. 11, No. 5/6, s. 383–396.
36. Roszak S., Kowal M., Góra R.: *The influence of the detachment of electrons on the properties and the nature of interactions in  $XH_2O$  ( $X = Cl, Br$ ) complexes*. *Journal of Chemical Physics*. 2001, Vol. 115, No. 8, s. 3469–3473.
37. Skarżewski J., Zielińska-Błajet M., Turowska-Tyrk I.: *Simple preparation of enantiometric Michael adducts of thiophenol to chalcones: easily available new chiral building*. *Tetrahedron: Asymmetry*. 2001, Vol. 12, No. 13, s. 1923–1928.
38. Sokalski A., Góra R., Bartkowiak W., Kobylński P., Sworakowski J., Chyla A., Leszczynski J.: *New theoretical insight into the thermal cis-trans isomerization of azo compounds: protonation lowers the activation barrier*. *Journal of Chemical Physics*. 2001, Vol. 114, No. 13, s. 5504–5508.
39. Sokalski A., Kędzierski P., Grembecka J.: *Ab initio study of the physical nature of interactions between enzyme active site fragments in vacuo*. *Physical Chemistry Chemical Physics*. 2001, Vol. 3, No. 5, s. 657–663.
40. Sołoducho J., Roszak S., Chyla A., Tajchert K.: *Synthetic routes to bis(pyrrolyl)arylenes: Experimental and molecular modeling studies*. *New Journal of Chemistry*. 2001, Vol. 25, No. 9, s. 1175–1181.
41. Stankowski J., Luty T., Kempniński W., Piekara-Sady L.: *Possible explanation of unstable superconducting phase in  $K_xC_{60}$  with  $T_c = 21$  K*. *Solid State Sciences*. 2001, Vol. 3, s. 531–537.
42. Strasburger K.: *Adiabatic positron affinity of LiH*. *Journal of Chemical Physics*. 2001, Vol. 114, No. 2, s. 615–616.
43. Sworakowski J., Janus K., Nešpůrek S.: *Kinetics of photochemical reactions in condensed phases: What can be borrowed from methods of dielectric physics*. *IEEE Transactions on Dielectrics and Electrical Insulation*. 2001, Vol. 8, No. 3, s. 543–548.
44. Turowska-Tyrk I.: *Structural transformations in a crystal during the photochemical reaction of 2-benzyl-5-benzylidenecyclopentanone*. *Chemistry: a European Journal*. 2001, Vol. 7, No. 15, s. 3401–3405.

45. Urban J., Roszak S., Leszczynski J.: *Shellvation of the ammonium cation by molecular hydrogen: a theoretical study*. Chemical Physics Letters. 2001, Vol. 346, No. 5/6, s. 512–518.
46. Videnova-Adrabińska V., Turowska-Tyrk I., Borowiak T., Dutkiewicz G.: *Topochemical bias in the hydrogen-bonded networks of guanidinium carboxybenzenesulfonates*. New Journal of Chemistry. 2001, Vol. 25, No. 11, s. 1403–1409.
47. Wójcik G., Holband J.: *Variable temperature crystal structure studies of m-nitroaniline*. Acta Crystallographica B. 2001, Vol. 57, pt. 3, s. 346–352.
48. Zhivkov I., Nešpůrek S., Sworakowski J.: *Trapping of charge carriers in organic molecular materials: phthalocyanine thin films revisited*. Acta Physica Polonica A. 2001, Vol. 100, suppl., s. 215–228.
49. Ziora Z., Kafarski P., Holband J., Wójcik G.: *Synthesis and spectroscopic characterization of protected N-phosphonomethylglycine dipeptides*. Journal of Peptide Science. 2001, Vol. 7, No. 9, s. 466–473.

## 2000

1. Bartkiewicz S., Miniewicz A., Kajzar F.: *Incoherent-to coherent image converter based on hybrid liquid crystal – photoconducting polymer structure*. Synthetic Metals. 2000, Vol. 109, No. 1–3, s. 105–108.
2. Bartkowiak W., Misiaszek T.: *Solvent effect on static vibrational and electronic contribution of first-order hyperpolarizability of pi-conjugated push-pull molecules: quantum-chemical calculations*. Chemical Physics. 2000, Vol. 261, No. 3, s. 353–357.
3. Bartkowiak W.: *Theoretical study of hyperpolarizabilities of aminobenzodifuranone*. Synthetic Metals. 2000, Vol. 109, No. 1–3, s. 109–111.
4. Dai D., Roszak S., Balasubramanian K.: *Electronic states and potential energy surfaces of NbC<sub>2</sub>*. Journal of Physical Chemistry A. 2000, Vol. 104, No. 24, s. 5861–5866.
5. Dai D., Roszak S., Balasubramanian K.: *Electronic structures of niobium carbides: NbC<sub>n</sub> (n = 3–8)*. Journal of Physical Chemistry A. 2000, Vol. 104, No. 43, s. 9760–9769.
6. Fabiański R., Kuchta B., Firlej L., Eters R.D.: *Calculations on the stability of low temperature solid nitrogen phases*. Journal of Chemical Physics. 2000, Vol. 112, No. 15, s. 6745–6748.

7. Fabiański R., Kuchta B., Firlej L.: *Computer calculations of stability of C<sub>70</sub> fullerene intercalated by alkali metals*. Synthetic Metals. 2000, Vol. 109, No. 1–3, s. 133–137.
8. Góra R., Roszak S., Leszczynski J.: *Properties and nature of interactions in CT(H<sub>2</sub>O)<sub>n</sub> (n = 1, 6) clusters: a theoretical study*. Chemical Physics Letters. 2000, Vol. 325, No. 1–3, s. 7–14.
9. Góra R., Roszak S., Leszczynski J.: *The electron affinity properties of NO(N<sub>2</sub>O)<sub>n</sub><sup>-</sup> (n = 1, 2) complexes*. Asian Journal of Spectroscopy. 2000, Vol. 4, No. 1, s. 1–9.
10. Jabłonka S., Mora C., Nowak P.M, Zaleski A: *The influence of some stabilizers on the sensitivity of AgBr(I) core-shell crystals*. Journal of Information Recording. 2000, Vol. 25, s. 603–609.
11. Jemmis E.D., Subramanian G., Nowek A., Góra R., Sullivan R.H., Leszczynski J.: *C-H...π interactions involving acetylene: an ab initio MO study*. Journal of Molecular Structure. 2000, Vol. 556, s. 315–320.
12. Kaczorowska M., Roszak S., Leszczynski J.: *The structure and properties of H<sub>3</sub><sup>+</sup>Ar<sub>n</sub> (n = 1–9) cations*. Journal of Chemical Physics. 2000, Vol. 113, No. 9, s. 3615–3620.
13. Kaplan I.G., Roszak S., Leszczynski J.: *Nature of binding in the alkaline-earth clusters: Be<sub>3</sub>, Mg<sub>3</sub>, and Ca<sub>3</sub>*. Journal of Chemical Physics. 2000, Vol. 113, No. 15, s. 6245–6252.
14. Kędzierski P., Sokalski A., Krauss M.: *Nonempirical analysis of nature of catalytic effects in ribonuclease A active site*. Journal of Computational Chemistry. 2000, Vol. 21, No. 6, s. 432–445.
15. Komorowska K., Miniewicz A., Parka J.: *Holographic grating recording in large area photoconducting liquid crystal panels*. Synthetic Metals. 2000, Vol. 109, No. 1–3, s. 189–193.
16. Luty T., Rohleder K., Lefebvre J., Descamps M.: *Supercooled plastic crystals as frustrated elastic domains: phenomenological theory for cyanoadamantane-family crystals*. Physical Review B. 2000, Vol. 62, No. 13, s. 8835–8843.
17. Miniewicz A., Komorowska K., Koval'chuk O.V., Vanhanen J., Sworakowski J., Kurik M.V.: *Studies of photorefractive properties of a novel dye-doped nematic liquid crystal system*. Advanced Materials for Optics and Electronics. 2000, Vol. 10, No. 2, s. 55–67.
18. Miniewicz A., Sikorski P., Januszko A., Bartkiewicz S., Parka J., Kajzar F.: *Optical image correlators based on nematic liquid crystals*. Nonlinear Optics. 2000, Vol. 25, s. 213–218.

19. Misiaszek T., Szostak M.M.: *Atomic charge distribution in 4-isopropylphenol molecule derived from atomic polar tensor*. Journal of Molecular Structure. 2000, Vol. 526, No. 1–3, s. 303–308.
20. Mora C., Czarniecka-Stefańska A.: *The modification of the crystals surface structure by epitaxial growth*. Journal of Information Recording. 2000, Vol. 25, s. 587–596.
21. Neal T.J., Kang S.-J., Turowska-Tyrk I., Schulz C.E., Scheidt R.W.: *Magnetic interactions in the high-spin iron(III) oxooctaethylchlorinato derivative, [Fe(oxoOEC)(Cl)], and its pi-cation radical, [Fe(oxoOEC)(Cl)]SbCl<sub>6</sub>*. Inorganic Chemistry. 2000, Vol. 39, No. 5, s. 872–880.
22. Nowak P.M.: *The relationship between granularity and light-sensitivity of the colour photographic materials*. Journal of Information Recording. 2000, Vol. 25, s. 567–585.
23. Osiadacz J., Majka J., Czarnecki K., Peczyńska-Czoch W., Zakrzewska-Czerwińska J., Kaczmarek Ł., Sokalski A.: *Sequence-selectivity of 5,11-dimethyl-5H-indolo[2,3-b]quinoline binding to DNA: Footprinting and molecular modeling studies*. Bioorganic & Medicinal Chemistry. 2000, Vol. 8, No. 5, s. 937–943.
24. Pawlik G., Mituś A., Miniewicz A.: *Monte-Carlo simulations of refractive index changes in nematic liquid crystal upon spatially nonuniform illumination*. Optics Communications. 2000, Vol. 182, No. 1–3, s. 249–254.
25. Rajkowski B., Nowak Piotr M.: *Modelling of acutance dye influence on the image sharpness in heterogenic light-sensitive layers*. Optica Applicata. 2000, Vol. 30, No. 2/3, s. 375–381.
26. Roszak S., Babinec P., Leszczynski J.: *New phenomena revealed by quantum chemical studies – the shellvation of GeH<sub>3</sub><sup>+</sup> by H<sub>2</sub> molecules*. Chemical Physics. 2000, Vol. 256, No. 2, s. 177–183.
27. Roszak S., Krauss M., Alekseyev A.B, Liebermann H., Buenker R.J.: *Spin-orbit configuration interaction calculation of the potential energy curves of iodine oxide*. Journal of Physical Chemistry A. 2000, Vol. 104, No. 13, s. 2999–3003.
28. Roszak S., Leszczynski J.: *The structure and nature of interactions in carbonium ions, CH<sub>3</sub><sup>+</sup>(H<sub>2</sub>)<sub>n</sub> (n = 1–9): a theoretical study*. Chemical Physics Letters. 2000, Vol. 323, No. 3/4, s. 278–286.
29. Ryley S., Chyla A., Peterson I.R.: *An air-stable biomimetic Langmuir-Blodgett bilayer*. Thin Solid Films. 2000, Vol. 370, No. 1/2, s. 294–298.
30. Strasburger K.: *Why Hylleraas-type functions failed to predict the existence of PsLi<sup>+</sup> and (2,3) PsHe<sup>+</sup>?*. International Journal of Quantum Chemistry. 2000, Vol. 79, No. 4, s. 243–252.

31. Sworakowski J.: *Effect of dipolar arrays on the localization of charge carriers in molecular materials*. IEEE Transactions on Dielectrics and Electrical Insulation. 2000, Vol. 7, No. 4, s. 531–536.
32. Wallenborn E.-U., Leontidis E., Palewska K., Suter U.W., Wild U.P.: *The Shpol'skii system perylene in n-hexane: a computational study of inclusion sites*. Journal of Chemical Physics. 2000, Vol. 112, No. 4, s. 1995–2002.
33. Walton D.J., Phull S.S., Geissler U., Chyla A., Durham A., Ryley S., Mason T.J., Lorimer J.P.: *Sonoelectrochemistry – cyclohexanoate electrooxidation at 38 kHz and 850 kHz insonation frequencies compared*. Electrochemistry Communications. 2000, Vol. 2, No. 6, s. 431–435.
34. Wyrzykiewicz E., Błaszczuk A., Turowska-Tyrk I.: *N-(E)-2-stilbenyloxymethylene-carbonyl substituted hydrazones of ortho, meta and para hydroxybenzaldehydes*. Bulletin of the Polish Academy of Sciences. Chemistry. 2000, Vol. 48, No. 3, s. 213–229.
35. Zaleski A., Jabłonka S., Mora C., Nowak P.M.: *The comparison of the sensitivity of AgBr(I) core-shell crystals with the crystals of homogeneous AgI distribution*. Journal of Information Recording. 2000, Vol. 25, s. 597–602.
36. Zych T., Turowska-Tyrk I., Lis T.: *Lithium phosphoenolpyruvate monohydrate at 85 K*. Acta Crystallographica C. 2000, Vol. 56, pt. 7, s. 818–819.

## 1999

1. Ashwell G.J., Skjonnemand K., Roberts M.P.S., Allen D.W., Li X., Sworakowski J., Chyla A., Bieńkowski M.: *Surface plasmon resonance and nonlinear optical studies of Langmuir-Blodgett films of a betaine dye*. Colloids and Surfaces A. 1999, Vol. 155, No. 1, s. 43–46.
2. Chyla A., Lorenz K., Chyla M.: *Mercury level in feathers of sparrows from industrial and nonindustrial areas of Lower Silesia, Poland: toward a non-destructive bioindicator of environmental pollution*. Environment Protection Engineering. 1999, Vol. 25, No. 4, s. 71–76.
3. Dai D., Roszak S., Balasubramanian K.: *Electronic states of the hafnium trimer ( $Hf_3$ )*. Chemical Physics Letters. 1999, Vol. 308, No. 5/6, s. 495–502.
4. Even J., Bertault M., Toupet L., Girard A., Kusto W.: *High temperature phase transitions in the crystal of p-trimethylammoniumbenzenesulfonate zwitterion*. European Physical Journal B. 1999, Vol. 12, No. 4, s. 479–491.

5. Even J., Bertault M., Toupet L., Kusto W.: *Ferroelastic domains and mechanical hysteresis in the crystal of p-(trimethylammonium) benzenesulphonate zwitterion*. Journal of Physics. 1999, Vol. 11, No. 30, s. 5797–5810.
6. Góra R., Roszak S., Leszczynski J.: *Structure and nature of interaction of the  $CH_3N_2^+$  ion by  $H_2$  molecules:  $CH_3N_2^+(H_2)_n$ ,  $n = 1-9$* . Journal of Physical Chemistry A. 1999, Vol. 103, No. 45, s. 9138–9143.
7. Graja A., Lipiec R., Waplak S., Król S., Turowska-Tyrk I., Drichko N.V.: *Interplay of acceptor molecule shape, crystal structure and physical properties of a new molecular complex  $C_{70} \cdot 2[(Ph_3P)AuCl]$* . Chemical Physics Letters. 1999, Vol. 313, No. 5/6, s. 725–732.
8. Grembecka J., Kędziński P., Sokalski A.: *Non-empirical analysis of the nature of the inhibitor-active-site interactions in leucine aminopeptidase*. Chemical Physics Letters. 1999, Vol. 313, No. 1/2, s. 385–392.
9. Janus K., Sworakowski J., Olszowski A., Lewanowicz A., Lipiński J., Luboch E., Biernat J.: *Kinetics of a photochromic reaction in a dibenzoazo crown ether in solution and in polymer matrices*. Advanced Materials for Optics and Electronics. 1999, Vol. 9, No. 5, s. 181–187.
10. Jones R., Krier A., Davidson K., Schmit J.P.N., Zawadzka J.: *Conductivity mechanisms in poly(p-phenylene vinylene) light-emitting diodes at high and low bias*. Thin Solid Films. 1999, Vol. 340, No. 1/2, s. 221–229.
11. Kaczmarek Ł., Peczyńska-Czoch W., Osiadacz J., Mordarski M., Sokalski A., Boratyński J., Marcinkowska E., Glazman-Kuśnierczyk H., Radzikowski C.: *Synthesis, and cytotoxic activity of some novel indolo[2,3-b]quinoline derivatives: DNA topoisomerase II inhibitors*. Bioorganic & Medicinal Chemistry. 1999, Vol. 7, No. 11, s. 2457–2464.
12. Kajzar F., Bartkiewicz S., Miniewicz A.: *Optical amplification with high gain in hybrid-polymer-liquid-crystal structures*. Applied Physics Letters. 1999, Vol. 74, No. 20, s. 2924–2926.
13. Kapała J., Rutkowska I., Roszak S., Miller M.: *Mass spectrometric and theoretical study of the mixed complex  $NaNdCl_4(g)$* . Polyhedron. 1999, Vol. 18, No. 22, s. 2845–2851.
14. Komorowska M., Lamperski J., Komorowski L.: *Near-infrared-induced proton transfer studied by electron spin resonance*. Chemical Physics. 1999, Vol. 244, No. 1, s. 101–109.

15. Koshihara S.Y., Takahashi Y., Sakai H., Tokura Y., Luty T.: *Photoinduced cooperative charge transfer in low-dimensional organic crystals*. Journal of Physical Chemistry B. 1999, Vol. 103, No. 14, s. 2592–2600.
16. Kuchta B., Descamps M., Willart J.F.: *Reducing quasi-ergodicity in Monte Carlo simulations of the plastic phase of the cyanoadamantane crystal*. Chemical Physics. 1999, Vol. 243, No. 1/2, s. 169–177.
17. Kuchta B., Firlej L.: *A model Monte Carlo simulations of the stability of hcp/fcc structures of C<sub>60</sub> and C<sub>70</sub> fullerene crystals*. Synthetic Metals. 1999, Vol. 103, No. 1–3, s. 2428–2429.
18. Kusto W., Bertault M., Even J.: *Thermal solid-state reaction of methyl p-dimethylaminobenzenesulfonate to trimethylammoniumbenzenesulfonate zwitterion: optical crystallographic studies*. Journal of Physical Chemistry B. 1999, Vol. 103, No. 47, s. 10549–10552.
19. Legendziewicz J., Keller B., Wojciechowski W., Turowska-Tyrk I.: *Synthesis, optical and magnetic properties of homo- and heteronuclear systems and glasses containing them*. New Journal of Chemistry. 1999, Vol. 23, No. 11, s. 1097–1103.
20. Lewanowicz A., Lipiński J., Nešpůrek S., Olszowski A., Śliwińska E., Sworakowski J.: *Photochromic activity of dihydropyridine derivatives: energetics and kinetics of photochemically driven reactions in polycrystalline 1-methyl-2,4,4,6-tetraphenyl-1,4-dihydropyridine*. Journal of Photochemistry and Photobiology A. 1999, Vol. 121, No. 2, s. 125–132.
21. Lipiński J., Bartkowiak W.: *Conformation and solvent dependence of the first and second molecular hyperpolarizabilities of charge-transfer chromophores: quantum-chemical calculations*. Chemical Physics. 1999, Vol. 254, s. 263–276.
22. Luty T., Eckhardt C.J., Lefebvre J.: *Langmuir monolayers as disordered solids: disorder and elastic fluctuations in mesophases*. Journal of Chemical Physics. 1999, Vol. 111, No. 22, s. 10321–10329.
23. Luty T., Swanson D., Eckhardt C.J.: *Langmuir monolayers as disordered solids: strain-tilt backbone coupling and natural order parameters for the swiveling transitions*. Journal of Chemical Physics. 1999, Vol. 110, No. 5, s. 2606–2611.
24. Munro O.Q., Serth-Guzzo J.A., Turowska-Tyrk I., Mohanrao K., Shokhireva T.K., Walker A.F., Debrunner P.G., Scheidt R.W.: *Two crystalline forms of low-spin [Fe(TMP)(5-MeHIm)<sub>2</sub>]ClO<sub>4</sub>: Relative parallel and perpendicular axial ligand orientations*. Journal of the American Chemical Society. 1999, Vol. 121, No. 44, s. 11144–11155.

25. Rajkowski B., Nowak P.M.: *Numerical investigation of sharpness in photographic layers containing DIR compounds*. *Optica Applicata*. 1999, Vol. 29, No. 3, s. 227–283.
26. Roszak S., Góra R., Leszczynski J.: *A theoretical study of the structures and energetics of  $O-Ar_n$  ( $n = 1-6$ ) clusters*. *Chemical Physics Letters*. 1999, Vol. 313, No. 1/2, s. 198–204.
27. Roszak S., Leszczynski J.: *The structures, thermodynamics, and nature of interactions of silanium cations shellvated by molecular hydrogen,  $SiH_3^+ (H^2)_n$  ( $n = 1-11$ )*. *Chemical Physics Letters*. 1999, Vol. 314, No. 3/4, s. 333–340.
28. Roszak S., Majumdar D., Balasubramanian K.: *Theoretical studies of structures and energetics of benzene complexes with  $Nb^+$  and  $Nb_2^+$  cations*. *Journal of Physical Chemistry A*. 1999, Vol. 103, No. 29, s. 5801–5806.
29. Śliwińska E., Sworakowski J.: *Kinetics and energetics of solid state reactions in a photochromic dihydropyridine derivative*. *Advanced Materials for Optics and Electronics*. 1999, Vol. 9, No. 4, s. 167–174.
30. Strasburger K.: *Binding energy, structure and annihilation properties of the positron-LiH molecule complex, studied with explicitly correlated Gaussian functions*. *Journal of Chemical Physics*. 1999, Vol. 11, No. 23, s. 10555–10558.
31. Sworakowski J., Nešpůrek S., Lipiński J., Lewanowicz A.: *On the mechanism of bleaching reactions in a photochromic dihydropyridine derivative*. *Journal of Photochemistry and Photobiology A*. 1999, Vol. 129, No. 1/2, s. 81–87.
32. Sworakowski J.: *Effect of polar molecules on the transport and localization of charge carriers in molecular materials*. *Brazilian Journal of Physics*. 1999, Vol. 29, No. 2, s. 318–331.
33. Veyrat M., Ramasseul R., Turowska-Tyrk I., Scheidt R.W., Autret M., Kadish K.M., Marchon J.-C.: *Nickel(II) and zinc(II) meso-tetracyclohexylporphyrins: Structural and electronic effects induced by meso-cyclohexyl substitution in metalloporphyrins*. *Inorganic Chemistry*. 1999, Vol. 38, No. 8, s. 1772–1779.
34. Wójcik G., Szostak M.M., Misiaszek T., Pająk Z., Wąsicki J., Kołodziej H.A., Freundlich P.: *Thermally induced rearrangement of hydrogen-bonded helices in solid 4-isopropylphenol as studied by calorimetric, proton NMR, dielectric and near IR spectroscopic methods*. *Chemical Physics*. 1999, Vol. 249, No. 2/3, s. 201–213.

## 1998

1. Balawender R., Komorowski L., De Proft F., Geerlings P.: *Derivatives of molecular valence as a measure of aromaticity*. *Journal of Physical Chemistry A*. 1998, Vol. 102, No. 48, s. 9912–9917.

2. Balawender R., Komorowski L.: *Atomic Fukui function indices and local softness ab initio*. Journal of Chemical Physics. 1998, Vol. 109, No. 13, s. 5203–5211.
3. Bartkiewicz S., Kajzar F., Miniewicz A.: *On the light-induced photoconductivity mediated grating formation in liquid crystal cells*. Photonics Science News. 1998, Vol. 3, Iss. 2, s. 22–26.
4. Bartkiewicz S., Miniewicz A., Kajzar F., Zagórska M.: *Enhanced photorefractive effect in hybrid conducting polymer – liquid crystal structures*. Molecular Crystals and Liquid Crystals Science and Technology A. 1998, Vol. 322, s. 9–20.
5. Bartkiewicz S., Miniewicz A., Kajzar F., Zagórska M.: *Enhanced photorefractive effect in a hybrid photoconducting polymer-liquid crystal panel*. Photonics Science News. 1998, Vol. 3, Iss. 4, s. 10–14.
6. Bartkiewicz S., Miniewicz A., Kajzar F., Zagórska M.: *Observation of high gain in a liquid-crystal panel with photoconducting polymeric layers*. Applied Optics. 1998, Vol. 37, No. 29, s. 6871–6877.
7. Bartkiewicz S., Sikorski P., Miniewicz A.: *Optical image correlator realized with a hybrid liquid-crystal-photoconducting polymer structure*. Optics Letters. 1998, Vol. 23, No. 22, s. 1769–1771.
8. Bartkowiak W., Lipiński J.: *Conformation and solvent dependence of the first molecular hyperpolarizability of pyridinium-N-phenoxide betaine dyes: Quantum chemical calculations*. Journal of Physical Chemistry A. 1998, Vol. 102, No. 27, s. 5236–5240.
9. Bartkowiak W., Lipiński J.: *Finite-field calculations of the second-order hyperpolarizabilities gamma of molecules in solutions*. Chemical Physics Letters. 1998, Vol. 292, No. 1/2, s. 92–96.
10. Chojnacki H.: *Quantum chemical studies of the double proton transfer in oxalic acid dimer*. Polish Journal of Chemistry. 1998, Vol. 72, No. 2, s. 421–425.
11. Chyla A., Lorenz K., Renzoni A., Gaggi C.: *Content of heavy metals in livers, kidneys and muscles of game in south-west Poland*. Environment Protection Engineering. 1998, Vol. 24, No. 3/4, s. 31–40.
12. Chyla A., Ryley S., Walton D.J., Liu X., Chetwynd D.G.: *Effect of dopand counter-anion on tribological properties of polypyrrole*. Advanced Materials for Optics and Electronics. 1998, Vol. 8, No. 2, s. 87–91.
13. Descamps M., Willart J.F., Kuchta B., Affouard F.: *Metastable state in glassy crystal cyanoadamantane: experiments and simulations*. Journal of Non-Crystalline Solids. 1998, Vol. 235–237, s. 559–566.

14. Dziekoński P., Sokalski A., Kassab E., Allavena M.: *Electrostatic nature of catalytic effects resulting from Si $\Rightarrow$ Al substitutions in ZMS-5 zeolite*. Chemical Physics Letters. 1998, Vol. 288, No. 2–4, s. 538–544.
15. Eckhardt C.J., Luty T., Peachey N.: *Collective interactions and solid state reactivity*. Molecular Crystals and Liquid Crystals Science and Technology A. 1998, Vol. 313, s. 25–38.
16. Eters R.D., Kuchta B.: *The character of melting for simple molecules deposited on graphite*. Journal of Low Temperature Physics. 1998, Vol. 111, No. 3/4, s. 271–286.
17. Even J., Bertault M., Gallier J., Girard A., Delugeard Y., Ecolivet C., Beaufile S., Toupet L., Kusto W.: *Influence of chemical pressure and reaction-induced stress in solid-state reaction: lattice instability during the thermally enhanced reaction of MSE*. Molecular Crystals and Liquid Crystals Science and Technology A. 1998, Vol. 313, s. 135–144.
18. Firlej L., Kuchta B., Roszak S.: *NMR study of molecular dynamics in C60.2([(C<sub>6</sub>H<sub>5</sub>)<sub>3</sub>P]AuCl) crystal*. Synthetic Metals. 1998, Vol. 94, No. 1, s. 77–81.
19. Huskowska E., Turowska-Tyrk I., Legendziewicz J., Głowiak T.: *Two high and low symmetry europium complexes with L-proline: spectroscopy and structure*. Journal of Alloys and Compounds. 1998, Vol. 275–277, s. 852–858.
20. Jankowski A., Dobryczycki P., Lipiński J., Stefanowicz P.: *Excited-state proton transfer in hydroxynaphthaldehydes covalently bound to proteins*. Journal of Fluorescence. 1998, Vol. 8, No. 2, s. 103–113.
21. Kapała J., Roszak S., Rutkowska I., Miller M.: *Mass spectrometric and theoretical study of the mixed complex NaCeCl<sub>4(g)</sub>*. Chemical Physics. 1998, Vol. 238, No. 2, s. 221–229.
22. Kuchta B., Descamps M., Affouard F.: *A Monte Carlo study of metastable structures of cyanoadamantane crystal*. Journal of Chemical Physics. 1998, Vol. 109, No. 16, s. 6753–6763.
23. Kuchta B., Luty T.: *Phase transformation in locally anharmonic systems: Susceptibility approach to orientational instabilities in molecular solids*. Polish Journal of Chemistry. 1998, Vol. 72, No. 2, s. 426–432.
24. Kuncewicz-Kupczyk W., Kapała J., Roszak S., Miller M.: *The thermodynamic properties of the gaseous dimer of CdI<sub>2</sub>*. Journal of Chemical Physics. 1998, Vol. 108, No. 18, s. 7743–7746.
25. Latacz L., Nowak P.M.: *Computer modelling of modulation transfer function and characteristic curve of AgHal light-sensitivity layers containing a dye*. Optica Applicata. 1998, Vol. 28, No. 2, s. 155–160.

26. Latacz L., Nowak P.M.: *Modelling of the exposure distribution inside heterogeneous radiosensitive layers*. Optica Applicata. 1998, Vol. 28, No. 3, s. 183–190.
27. Lewanowicz A., Lipiński J., Siedlecka R., Skarżewski J., Baert F.: *Chiral beta-amino sulfoxides: Synthesis, configurational assignment and conformational analysis based on X-ray, CD, 1H NMR, and theoretical calculations*. Tetrahedron. 1998, Vol. 54, No. 23, s. 6571–6586.
28. Lewanowicz A., Lipiński J.: *Low-lying excited singlet states and S<sub>2</sub>-SO luminescence of dipyrido[3,4-b: 2,3-d]phenazine*. Journal of Molecular Structure. 1998, Vol. 450, No. 1–3, s. 163–169.
29. Miniewicz A., Bartkiewicz S., Kajzar F.: *On the dynamics of coherent amplification of light observed in liquid crystal panel with photoconducting polymeric layers*. Molecular Crystals and Liquid Crystals Science and Technology B. 1998, Vol. 19, No. 2, s. 157–175.
30. Miniewicz A., Bartkiewicz S., Parka J.: *Optical phase conjugation in dye-doped nematic liquid crystal*. Optics Communications. 1998, Vol. 149, No. 1–3, s. 89–95.
31. Miniewicz A., Bartkiewicz S., Sworakowski J., Giacometti J.A., Costa M.M.: *On the optical phase conjugation in polystyrene films containing azobenzene dye Disperse Red 1*. Pure and Applied Optics. 1998, Vol. 7, No. 4, s. 709–721.
32. Miniewicz A., Delysse S., Nunzi J.-M., Kajzar F.: *Two-photon absorption resonance in 3-(1,1-dicyanoethenyl)-1-phenyl-4,5-dihydro-1H-pyrazole (DCNP)*. Chemical Physics Letters. 1998, Vol. 287, No. 1/2, s. 17–21.
33. Miniewicz A., Parka J., Bartkiewicz S., Januszko A.: *Liquid crystals as materials for real-time holographic optical devices*. Pure and Applied Optics. 1998, Vol. 7, No. 2, s. 179–189.
34. Nowak P.M.: *Modelling of the modulation transfer function of silver halide light – sensitive layer including DIR and DAR dye couplers*. Optica Applicata. 1998, Vol. 28, No. 2, s. 95–104.
35. Ordon P., Komorowski L.: *Nuclear reactivity and nuclear stiffness in density functional theory*. Chemical Physics Letters. 1998, Vol. 292, No. 1/2, s. 22–27.
36. Rajkowski B., Nowak P.M.: *Model investigation of the influence of adjacency edge effects on the shape and properties of the limiting curve in the silver halide light – sensitive materials*. Optica Applicata. 1998, Vol. 28, No. 2, s. 105–113.
37. Roszak S., Balasubramanian K.: *Structural and thermodynamic properties of diyttrium carbides Y<sub>2</sub>C<sub>n</sub> (n = 2–8): a theoretical study*. Journal of Physical Chemistry A. 1998, Vol. 102, No. 29, s. 6004–6009.

38. Skipirzepski P., Nowak P.M.: *Optimization of the optical granularity measurement conditions of model photographic layers*. *Optica Applicata*. 1998, Vol. 28, No. 3, s. 173–181.
39. Strasburger K., Chojnacki H.: *Quantum chemical study of simple positronic systems using explicitly correlated Gaussian functions  $PsH$  and  $PsLi^+$* . *Journal of Chemical Physics*. 1998, Vol. 108, No. 8, s. 3218–3221.
40. Sworakowski J., Lipiński J., Palewska K., Nešpůrek S., Ziółek Ł.: *Effect of the substituents on the solvatochromic behaviour of benzimidazole-based betaine dyes*. *Journal of Molecular Structure*. 1998, Vol. 471, No. 1–3, s. 27–35.
41. Sworakowski J., Nešpůrek S., Bertault M.: *Thermally stimulated technique employed to reactions in polycrystalline photochromic systems*. *Molecular Crystals and Liquid Crystals Science and Technology A*. 1998, Vol. 313, s. 199–204.
42. Sworakowski J., Nešpůrek S.: *„Fractional heating” differential scanning calorimetry: a tool to study energetics and kinetics of solid-state reactions in photoactive systems with distributed parameters*. *Chemical Physics*. 1998, Vol. 238, No. 2, s. 343–351.
43. Sworakowski J., Nešpůrek S.: *A straightforward method of analysis of first-order process with distributed parameters*. *Chemical Physics Letters*. 1998, Vol. 298, No. 1–3, s. 21–26.
44. Sworakowski J., Nešpůrek S.: *Contribution of dipolar species to the formation of local states for charge carriers in molecular materials*. *Polish Journal of Chemistry*. 1998, Vol. 72, No. 2, s. 163–171.
45. Szostak M.M., Kozankiewicz B., Wójcik G., Lipiński J.: *Photoluminescence and quantum chemical studies of electronic and optical properties of *m*-nitroaniline and *m*-nitrophenol crystals*. *Journal of the Chemical Society. Faraday Transactions*. 1998, Vol. 94, No. 21, s. 3241–3245.
46. Szostak M.M., Wójcik G., Gallier J., Bertault M., Freundlich P., Kołodziej H.A.:  *$^1H$ -NMR, dielectric and calorimetric studies of molecular motions in *m*-nitroaniline crystal*. *Chemical Physics*. 1998, Vol. 229, No. 2/3, s. 275–284.
47. Turalski W., Miniewicz A.: *Calculations of electric field dependence of effective refractive index in nematic liquid crystal panel*. *Molecular Crystals and Liquid Crystals Science and Technology A*. 1998, Vol. 325, s. 117–126.

**1997**

1. Balawender R., Komorowski L., Roszak S.: *Acidic and basic molecular hardness in LCAO approximation*. International Journal of Quantum Chemistry. 1997, Vol. 61, No. 3, s. 499–505.
2. Bieńko D.C., Michalska D., Roszak S., Wojciechowski W., Nowak M.J., Łapiński L.: *Infrared matrix isolation and theoretical studies on glutarimide*. Journal of Physical Chemistry A. 1997, Vol. 101, No. 42, s. 7834–7841.
3. Cailleau H., Lemee-Cailleau M.H., Le Cointe M., Luty T.: *Physics of neutral-to-ionic phase transition in organic charge transfer semiconducting*. Acta Physica Polonica A. 1997, Vol. 92, No. 4, s. 597–608.
4. Chojnacki H.: *Correlation effects in the double proton transfer of the formic acid dimer*. Molecular Engineering. 1997, Vol. 7, s. 161–167.
5. Chojnacki H.: *Correlation effects in the proton transfer of the  $[FHF]^{(-)}$  system*. Journal of Molecular Structure. 1997, Vol. 404, No. 1/2, s. 83–85.
6. Dobrzyńska D., Turowska-Tyrk I.: *9,10-dihydro-9-oxo-10-acridineacetic acid*. Acta Crystallographica C. 1997, Vol. 53, pt. 2, s. 238–239.
7. Even J., Bertault M., Gallier J., Girard A., Delugeard Y., Kusto W.: *Evidence of a lattice instability during the thermally enhanced reaction of MSE studied by calorimetry,  $C^{13}$ -NMR, Raman scattering and birefringence*. Chemical Physics Letters. 1997, Vol. 279, No. 5/6, s. 319–326.
8. Koski W.S., Roszak S., Kaufman J.J., Balasubramanian K.: *Potential toxicity of  $CF_3X$  halocarbons*. In Vitro Toxicology. 1997, Vol. 10, No. 4, s. 455–457.
9. Kuchta B., Rohleder K., Swanson D., Eters R.D.: *A calculation of the entropy and free energy differences between the alpha and beta phases of solid nitrogen*. Journal of Chemical Physics. 1997, Vol. 106, No. 16, s. 6771–6773.
10. Lemee-Cailleau M.H., Le Cointe M., Cailleau H., Luty T., Moussa F., Roos J., Brinkmann D., Toudic B., Ayache C., Karl N.: *Thermodynamics of the neutral-to-ionic transition as condensation and crystallization of charge-transfer excitations*. Physical Review Letters. 1997, Vol. 79, No. 9, s. 1690–1693.
11. Lipiński J., Bartkowiak W.: *Solvent effect on the electronic structure of molecules studies by the Langevin dipoles/Monte Carlo approach*. Journal of Physical Chemistry A. 1997, Vol. 101, No. 11, s. 2159–2165.

12. Majumdar D., Roszak S., Balasubramanian K.: *Theoretical study of the interaction of benzene with  $Rh^+$  and  $Rh_2^+$  cations*. Journal of Chemical Physics. 1997, Vol. 107, No. 2, s. 408–414.
13. Mergulhao S., Faria R.M., Leal F.G., Sworakowski J.: *Transport of holes uniformly and non-uniformly protonated poly(o-methoxyaniline)*. Chemical Physics Letters. 1997, Vol. 269, No. 5/6, s. 489–493.
14. Roszak S., Balasubramanian K.: *Electronic structure and thermodynamic properties of  $ScC_2$* . Journal of Physical Chemistry A. 1997, Vol. 101, No. 14, s. 2666–2669.
15. Roszak S., Balasubramanian K.: *Potential energy surfaces for the  $Ta^+ + C_2$  reaction*. Journal of Chemical Physics. 1997, Vol. 106, No. 10, s. 4008–4012.
16. Roszak S., Balasubramanian K.: *Stabilities of isomers of  $LaC_{12}^+$  and  $LaC_{13}^+$* . Chemical Physics Letters. 1997, Vol. 264, No. 1/2, s. 80–84.
17. Roszak S., Balasubramanian K.: *Theoretical investigation of structural and thermodynamic properties of lanthanum carbides  $LaC_n$  ( $n = 2-6$ )*. Journal of Chemical Physics. 1997, Vol. 106, No. 1, s. 158–164.
18. Roszak S., Balasubramanian K.: *Theoretical study of the isomerization of  $TaC_n^+$  ( $n = 7-13$ ) cations*. Chemical Physics Letters. 1997, Vol. 265, No. 3–5, s. 553–560.
19. Roszak S., Koski W.S., Kaufman J.J., Balasubramanian K.: *Structure and energetics of  $CF_3Cl^-$ ,  $CF_3Br^-$ , and  $CF_3I^-$  radical anions*. Journal of Chemical Physics. 1997, Vol. 106, No. 18, s. 7709–7713.
20. Roszak S., Rzepiela A.: *The structure, proton affinity, electrostatic properties and its relation to biological activity of cocaine and its derivatives*. Computational Methods in Science and Technology. 1997, Vol. 3, s. 55–62.
21. Schulz L., Chojnacki H.: *Structure and phenomenon relationships – a theoretical study*. Journal of Molecular Structure. 1997, Vol. 404, No. 1/2, s. 87–90.
22. Swanson D., Luty T., Eckhardt C.J.: *Langmuir monolayers as disordered solids: strain-state calculations applied to stearic acid*. Journal of Chemical Physics. 1997, Vol. 107, No. 12, s. 4744–4750.
23. Turalski W., Miniewicz A., Mituś A.: *Monte Carlo simulation of the Fredericksz transition in nematic liquid crystals*. Advanced Materials for Optics and Electronics. 1997, Vol. 7, No. 2, s. 71–77.
24. Turalski W., Mituś A., Miniewicz A.: *Monte Carlo simulation of electric-field-induced spatial gratings in nematic liquid crystals*. Pure and Applied Optics. 1997, Vol. 6, s. 589–598.

**1996**

1. Bartkiewicz S., Januszko A., Miniewicz A., Parka J.: *Dye-doped liquid crystal composite for real-time holography*. Pure and Applied Optics. 1996, Vol. 5, No. 6, s. 799–809.
2. Bartkiewicz S., Miniewicz A.: *Mechanism of optical recording in doped liquid crystals*. Advanced Materials for Optics and Electronics. 1996, Vol. 6, No. 5/6, s. 219–224.
3. Bartkiewicz S., Miniewicz A.: *Molecular systems for real time holography*. Molecular Physics Reports. 1996, Vol. 14, s. 59–67.
4. Bartkowiak W., Lipiński J.: *Studies of the solvent effect on the molecular hyperpolarisabilities of organic molecules*. Advanced Materials for Optics and Electronics. 1996, Vol. 6, No. 5/6, s. 248–254.
5. Bourges P., Lemee-Cailleau M.H., Launois P., Ecolivet C., Cailleau H., Moussa F., Mierzejewski A.: *Pretransitional dynamics of the structural phase transition in anthracene-TCNB: a comparison of Raman-scattering and inelastic-neutron-scattering experiments*. Physical Review B. 1996, Vol. 54, No. 21, s. 15002–15015.
6. Chyla A., Lorenz K., Gaggi C., Renzoni A.: *Pollution effects on wildlife: roe deer antlers as non-destructive bioindicator*. Environment Protection Engineering. 1996, Vol. 22, No. 3/4, s. 65–70.
7. Dai D., Roszak S., Balasubramanian K.: *Theoretical study of potential energy surfaces for interactions of Pd<sub>2</sub> with CO*. Journal of Chemical Physics. 1996, Vol. 104, No. 4, s. 1471–1476.
8. Fabiański R., Kuchta B.: *Theoretical energy minimisation and optimisation of structures of C60 fullerene compounds*. Advanced Materials for Optics and Electronics. 1996, Vol. 6, No. 5/6, s. 297–300.
9. Hamzaoui F., Baert F., Wójcik G.: *Electron-density study of m-nitrophenol in the orthorhombic structure*. Acta Crystallographica B. 1996, Vol. 52, pt. 1, s. 159–164.
10. Jabłonka S., Mora C., Nowak P.M., Zaleski A.: *Photographic testing method for reducing properties of gelatins*. Journal of Information Recording Materials. 1996, Vol. 23, No. 4, s. 309–313.
11. Jabłonka S., Mora C., Nowak P.M., Zaleski A.: *Some aspects of the action of tetraazaindene derivatives in the photographic process in AgBr(I) twin crystals*. Journal of Information Recording Materials. 1996, Vol. 23, No. 3, s. 249–254.

12. Jabłonka S., Mora C., Nowak P.M., Zaleski A.: *The influence of some organic compounds on the recrystallization of fine grain AgBr emulsions*. Journal of Information Recording Materials. 1996, Vol. 23, No. 4, s. 303–308.
13. Januszko A., Miniewicz A.: *Self-diffraction studies in a Se-nematic liquid crystal cell*. Advanced Materials for Optics and Electronics. 1996, Vol. 6, No. 5/6, s. 272–278.
14. Kaufman J.J., Koski W.S., Roszak S., Balasubramanian K.: *Correlation between energetics and toxicities of single-carbon halides*. Chemical Physics. 1996, Vol. 204, No. 2/3, s. 233–237.
15. Komorowski L., Boyd S.L., Boyd R.J.: *Electronegativity and hardness of disjoint and transferable molecular fragments*. Journal of Physical Chemistry. 1996, Vol. 100, No. 9, s. 3448–3453.
16. Kuchta B., Eters R.D.: *Melting behavior of quasi-two-dimensional N<sub>2</sub> adlayers deposited on graphite*. Physical Review B. 1996, Vol. 54, No. 17, s. 12057–12066.
17. Kuchta B., Roszak S., Eters R.D.: *Solid iodine under pressure: A study of intermolecular interactions*. Molecular Physics Reports. 1996, Vol. 14, s. 33–39.
18. Kuczera J., Chojnacki H., Kral T.E., Przystalski S.: *Effect of amphiphilic cationic compounds on calcium ion desorption from lecithin liposome membranes: Kinetic studies and quantum chemical calculations*. Zeitschrift für Naturforschung C. 1996, Vol. 51, No. 3/4, s. 219–225.
19. Lewanowicz A., Roszak S., Siedlecka R.: *The structural study of beta-amino sulfoxide*. Molecular Physics Reports. 1996, Vol. 14, s. 9–17.
20. Lewanowicz A., Siedlecka R., Bartkowiak W., Hamzaoui F.: *Sulphur-containing compounds: structure, spectra, non-linearity: Experimental and theoretical study*. Advanced Materials for Optics and Electronics. 1996, Vol. 6, No. 5/6, s. 225–232.
21. Lipiński J., Komorowski L.: *The solvent effect on the electro-negativity and hardness of bonded atoms*. Chemical Physics Letters. 1996, Vol. 262, No. 3/4, s. 449–454.
22. Luty T.: *Explosive molecular crystals: on the mechanism of detonation*. Molecular Physics Reports. 1996, Vol. 14, s. 157–167.
23. Luty T., Eckhardt C.J.: *Phase transitions in quasi-two-dimensional molecular solids: tilt-induced elastic multipoles and their interaction and ferroelasticity in Langmuir monolayers*. Journal of Physical Chemistry. 1996, Vol. 100, No. 16, s. 6793–6800.
24. Nowak P.M.: *Computation of the modulation transfer function of photographic materials by the edge function method*. Optica Applicata. 1996, Vol. 26, No. 2, s. 113–126.

25. Piecuch P., Tobała R., Paldus J.: *Approximate account of connected quadruply excited clusters in single-reference coupled-cluster theory via cluster analysis of the projected unrestricted Hartree-Fock wave function*. Physical Review. A. 1996, Vol. 54, No. 2, s. 1050–1241.
26. Przystalski S., Hładyszowski J., Kuczera J., Różycka-Roszak B., Trela Z., Chojnacki H., Witek S., Fiscicaro E.: *Interaction between model membranes and a new class of surfactants with antioxidant function*. Biophysical Journal. 1996, Vol. 70, No. 5, s. 2203–2211.
27. Rohleder K., Kuchta B.: *Monte Carlo simulations of alpha-beta transitions*. Molecular Physics Reports. 1996, Vol. 14, s. 153–156.
28. Roszak S., Balasubramanian K.: *Electronic structure and thermodynamic properties of YIrC and YIrC<sub>2</sub>*. Chemical Physics Letters. 1996, Vol. 254, No. 3/4, s. 274–280.
29. Roszak S., Balasubramanian K.: *Electronic structure and thermodynamic properties of LaC<sub>2</sub>*. Journal of Physical Chemistry. 1996, Vol. 100, No. 27, s. 11255–11259.
30. Roszak S., Balasubramanian K.: *Theoretical study of structural and thermodynamic properties of yttrium carbides, YC<sub>n</sub> (n = 2–6)*. Journal of Physical Chemistry. 1996, Vol. 100, No. 20, s. 8254–8259.
31. Roszak S.: *An ab initio configuration interaction study of deprotonation and dehydrogenation pathways of the hydronium cation*. Chemical Physics Letters. 1996, Vol. 250, No. 2, s. 187–191.
32. Roszak S.: *Theoretical study of properties of H<sup>(-)</sup> and NH<sub>2</sub><sup>(-)</sup> complexes with neutral ammonia solvent molecules*. Journal of Chemical Physics. 1996, Vol. 105, No. 17, s. 7569–7572.
33. Schulz L., Chojnacki H.: *Resemblance analysis of molecular systems on the grounds of DFT-evaluated parameters: Platinum complexes and their anticancer activity*. International Journal of Quantum Chemistry. Quantum Chemistry Symposium, 1996, No. 30, s. 173–179.
34. Strasburger K.: *Quantum chemical study on complexes of the LiH molecule with e<sup>+</sup>, Ps and Ps<sup>-</sup> including correlation energy*. Chemical Physics Letters. 1996, Vol. 253, No. 1/2, s. 49–52.
35. Sworakowski J., Goncalves D., Oliveira O.N. Jr, Faria R.M.: *Deposition and electrical conductivity of poly(o-methoxyaniline) Langmuir-Blodgett films*. Chemické Listy. 1996, Vol. 90, No. 1, s. 52–55.
36. Sworakowski J., Lipiński J., Ziótek Ł., Palewska K., Nešpůrek S.: *Solvatochromism of a zwitterionic benzimidazole-based pyridinium betaine dye: UV-Vis spec-*

- trosopic measurements and quantum-chemical calculations.* Journal of Physical Chemistry. 1996, Vol. 100, No. 30, s. 12288–12294.
37. Turalski W., Miniewicz A., Bartkiewicz S.: *On the dynamic self-diffraction in methylene blue-sensitized gelatine.* Advanced Materials for Optics and Electronics. 1996, Vol. 6, No. 1, s. 15–25.
38. Turalski W., Miniewicz A.: *Numerical modelling of space charge field in a photorefractive material illuminated by a nonsinusoidal light intensity pattern.* Optics Communications. 1996, Vol. 128, No. 4–6, s. 385–392.

## 1995

1. Balawender R., Gupta M., Orgaz E., Komorowski L.: *Electronic structure of  $KMgH_3$ ,  $KMgH_2F$ ,  $KMgF_3$  with the perovskite structure.* Acta Physica Polonica A. 1995, Vol. 88, No. 6, s. 1133–1141.
2. Bartkiewicz S., Miniewicz A.: *Dynamic self-diffraction studies in some dye-doped gelatins.* Pure and Applied Optics. 1995, Vol. 4, No. 6, s. 741–751.
3. Bartkiewicz S., Miniewicz A.: *Methylene blue sensitized poly(methyl methacrylate) matrix: a novel holographic material.* Applied Optics. 1995, Vol. 34, No. 23, s. 5175–5179.
4. Bartkiewicz S., Miniewicz A.: *On the nature of optical phase conjugation in methylene blue sensitized gelatin.* Molecular Crystals and Liquid Crystals Science and Technology B. 1995, Vol. 12, No. 3, s. 179–191.
5. Chojnacki H., Andzelm J., Nguyen D.T., Sokalski A.: *Preliminary density functional calculations on the formic acid dimer.* Computers and Chemistry. 1995, Vol. 19, No. 3, s. 181–187.
6. Heritier M., Charfi-Kaddour S., Ordon P.: *Properties of quasi-two-dimensional superconductors near a SDW instability: application to ET-salts.* Synthetic Metals. 1995, Vol. 70, No. 1–3, s. 1025–1026.
7. Komorowska M., Wójcik G., Szostak M.M.: *ESR studies of near infrared induced unpaired spins in two polymorphs of meta-nitrophenol.* Journal of Molecular Structure. 1995, Vol. 348, s. 445–448.
8. Kucharski S., Janik R., Bryjak M., Bieńkowski M., Chyla A., Sworakowski J.: *Formation and deposition of Langmuir films of binary and ternary systems.* Polish Journal of Chemistry. 1995, Vol. 69, No. 3, s. 447–460.
9. Kuchta B., Eters R.D.: *Free energy computer simulation in solid state chemistry.* Computers and Chemistry. 1995, Vol. 19, No. 3, s. 205–208.

10. Kuchta B., Rohleder K., Eters R.D., Belak J.: *A Monte Carlo study of the alpha-beta order-disorder transition in solid nitrogen*. Journal of Chemical Physics. 1995, Vol. 102, No. 8, s. 3349–3353.
11. Lefebvre J., Rohleder K., Mierzejewski A., Luty T.: *Structure, disorder, and phase transition in ternary crystals of anthracene, phenanthrene, and tetracyanobenzene,  $A_xPh_{(1-x)}TCNB$* . Journal of Chemical Physics. 1995, Vol. 102, No. 5, s. 2165–2173.
12. Lipiński J., Chojnacki H.: *Solvent effect on the spectroscopic properties of indole – semiempirical quantum chemical study*. Spectrochimica Acta A. 1995, Vol. 51, No. 3, s. 381–386.
13. Longeville S., Even J., Bertault M., Kołodziej H.A., Sworakowski J.: *Dielectric study of pure polymer and mixed monomer-polymer single crystals of pTS diacetylene: a comparison with neutron scattering results*. Acta Physica Polonica A. 1995, Vol. 88, No. 2, s. 359–367.
14. Luty T., Eckhardt C.J.: *General theoretical concepts for solid state reactions: quantitative formulation of the reaction cavity, steric compression, and reaction-induced stress using an elastic multipole representation of chemical pressure*. Journal of the American Chemical Society. 1995, Vol. 117, No. 9, s. 2441–2452.
15. Luty T., Eckhardt C.J.: *Phase transitions in quasi-two-dimensional molecular solids: A microscopic theory of tilt and structural instabilities in Langmuir monolayers*. Journal of Physical Chemistry. 1995, Vol. 99, No. 21, s. 8872–8887.
16. Luty T.: *Ground state phase diagram of mixed-stack compounds with intermolecular electron transfer*. Acta Physica Polonica A. 1995, Vol. 87, No. 6, s. 1009–1021.
17. Maślankiewicz A., Głowiak T., Chojnacki H., Skrzypek T., Niedbała A.: *X-Ray structure of isomeric 3-chloro-4-(methylthio)- and 4-chloro-3-(methylthio)quinolines*. Journal of Chemical Crystallography. 1995, Vol. 25, No. 4, s. 165–169.
18. Miniewicz A., Bartkiewicz S.: *Photosensitive guest-host polymer for optical data storage*. Acta Physica Polonica A. 1995, Vol. 87, No. 6, s. 971–980.
19. Miniewicz A., Żuk W., Jakubas R.: *Electro-optic coefficients of ferroelectric PMACB and PMABB crystals*. Ferroelectrics. 1995, Vol. 165, No. 3/4, s. 241–248.
20. Mulder A., Michels J.P.J., Schouten J.A., Kuchta B., Eters R.D.: *Monte Carlo calculations on the beta-delta phase transition in nitrogen with a generalized free energy method*. International Journal of Thermophysics. 1995, Vol. 16, No. 4, s. 957–963.

21. Nowak P.M., Mora C.: *A computer technique for the quality evaluation of the photographic image*. Journal of Information Recording Materials. 1995, Vol. 22, No. 3, s. 275–278.
22. Nowak P.M.: *Die Schaerfe des photographischen Bildes*. Journal of Information Recording Materials. 1995, Vol. 22, No. 3, s. 239–247.
23. Palewska K., Lipiński J., Sworakowski J., Sepioł J., Gygax H., Meister E.C., Wild U.P.: *Total luminescence spectroscopy of terylene in low-temperature Shpol'skii matrices*. Journal of Physical Chemistry. 1995, Vol. 99, No. 46, s. 16835–16841.
24. Piecuch P., Toboła R., Paldus J.: *Coupled-cluster approaches with an approximate account of triply and quadruply excited clusters: implementation of the orthogonally spin-adapted CCD + ST(CCD), CCSD + T(CCSD), and ACPQ + ST(ACPQ) formalisms*. International Journal of Quantum Chemistry. 1995, Vol. 55, No. 2, s. 133–146.
25. Radomski R., Radomska M., Dankowski M., Szajowska K., Wisiański Z.: *Micro-computer-controlled electrochemical universal meter*. Computers and Chemistry. 1995, Vol. 19, No. 3, s. 303–323.
26. Roszak S., Balasubramanian K.: *A theoretical study of bridged vs atop interactions of Pt<sub>2</sub> with CO*. Journal of Chemical Physics. 1995, Vol. 103, No. 3, s. 1043–1049.
27. Roszak S., Balasubramanian K.: *Theoretical study of structure and thermodynamic properties of YC<sub>2</sub>*. Chemical Physics Letters. 1995, Vol. 246, No. 1/2, s. 20–25.
28. Roszak S., Balasubramanian K.: *Theoretical study of the Diels-Alder reactions of zirconium dimer with ethylene and butadiene*. Journal of Physical Chemistry. 1995, Vol. 99, No. 11, s. 3487–3492.
29. Roszak S., Balasubramanian K.: *Theoretical study of the interaction of benzene with platinum atom and cation*. Chemical Physics Letters. 1995, Vol. 234, No. 1–3, s. 101–106.
30. Roszak S., Chojnacki H., Balasubramanian K.: *On symmetry-concerted organo-metallic analogues of the ethylene dimerization*. Acta Physica Polonica A. 1995, Vol. 87, No. 6, s. 965–969.
31. Samek L., Miniewicz A.: *Effect of nitrogen addition on optical properties of fluoro-zirconate glasses*. Advanced Materials for Optics and Electronics. 1995, Vol. 5, No. 5, s. 265–268.
32. Samoć M., Świątkiewicz J., Samoć A., Luther-Davies B., Olszowski A.: *Third-order nonlinear optical properties of pseudoazulenes*. Acta Physica Polonica A. 1995, Vol. 88, No. 2, s. 411–416.

33. Strasburger K., Chojnacki H.: *On the reliability of the SCF and CI wavefunctions for systems containing positrons*. Chemical Physics Letters. 1995, Vol. 241, No. 5/6, s. 485–489.
34. Strasburger K.: *A general program to calculate moments of the electron density distribution and multipolar interactions*. Computers and Chemistry. 1995, Vol. 19, No. 3, s. 259–261.
35. Sveleba S.A., Polovinko I.I., Bublyk M.I., Kusto W.: *Dvuluceprelomljajuscie svojstva nesorazmernych faz tipa „re-enter” v kristallach (C<sub>3</sub>H<sub>7</sub>NH<sub>3</sub>)<sub>2</sub>MeCl<sub>4</sub> (Me = Cu, Cd, Mn)*. Kristallografija. 1995, t. 40, No. 1, s. 104–112.
36. Szostak M.M., Misiaszek T., Roszak S., Rankin J.G., Czernuszewicz R.S.: *Experimental and theoretical studies of vibrational and electronic spectra of the molecule and crystal of p-isopropylphenol*. Journal of Physical Chemistry. 1995, Vol. 99, No. 41, s. 14992–15003.
37. Turalski W., Miniewicz A.: *A simple numerical simulation model for space charge field formation in photorefractive materials*. Journal of Applied Physics. 1995, Vol. 77, No. 4, s. 1554–1560.
38. Walton D.J., Phull S.S., Chyla A., Lorimer J.P., Mason T.J., Burke L.D., Murphy M., Compton R.G., Eklund J.C., Page S.D.: *Sonovoltammetry at platinum electrodes: surface phenomena and mass transport processes*. Journal of Applied Electrochemistry. 1995, Vol. 25, No. 12, s. 1083–1090.
39. Wójcik G., Giermańska J., Marqueton Y., Foulon M.: *Monotropic character of polymorphism in pentachloropyridine crystal studies by calorimetric and spectroscopic methods*. Acta Physica Polonica A. 1995, Vol. 88, No. 2, s. 339–347.
40. Wójcik G., Toupet L., Gors C., Foulon M.: *Crystal structures, phase transitions, and hydrogen bondings in pentabromophenol, pentachlorophenol, and their mixed crystals*. Physica Status Solidi A. 1995, Vol. 147, No. 1, s. 99–109.
41. Ziótek Ł., Palewska K., Lipiński J., Sworakowski J., Nešpůrek S., Bohm S., Meister E.C.: *Solvatochromic effect in a benzimidazole-based betaine: determination of the dipole moments and second-order hyperpolarizability*. Acta Physica Polonica A. 1995, Vol. 88, No. 2, s. 283–293.

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1. Bartkiewicz S., Chyla A., Sworakowski J., Janik R., Kucharski S.: *Deposition, electrical conductivity and response to gases of two-component Langmuir-Blodgett films containing pre-formed poly(3-n-alkylthiophenes)*. Polish Journal of Chemistry. 1994, Vol. 68, No. 7, s. 1387–1393.

2. Bourges P., Rabiller P., Mierzejewski A., Cailleau H., Lemee-Cailleau M.H., Ecolivet C., Moussa F.: *Crossover of the dynamical regime of the SPT in A-TCNB under hydrostatic pressure*. *Ferroelectrics*. 1994, Vol. 159, No. 14, s. 19–24.
3. Chojnacki H.: *Density functional studies on the double proton transfer in the formic acid dimer*. *Bulletin of the Polish Academy of Sciences. Chemistry*. 1994, Vol. 42, No. 4, s. 557–570.
4. Krauss M., Roszak S.: *Excited states of the phenyl radical*. *Journal of Molecular Structure. Theochem*. 1994, Vol. 116, s. 155–160.
5. Laforgue A., Guerin P., Roszak S.: *Determination of the correlation effects in molecules using the complete error potential*. *Theoretica Chimica Acta*. 1994, Vol. 88, No. 2, s. 117–129.
6. Luty T., Kuchta B., Rohleder K.: *Phenomenological theory of electron and methyl transfer reactions in organic crystals*. *Molecular Crystals and Liquid Crystals Science and Technology A*. 1994, Vol. 240, s. 259–267.
7. Miniewicz A., Jakubas R., Ecolivet C., Girard A.: *Raman scattering in ferroelectric  $(\text{CH}_3\text{NH}_3)_3\text{Bi}_2\text{Br}_9$  single crystals*. *Journal of Raman Spectroscopy*. 1994, Vol. 25, No. 5, s. 371–375.
8. Miniewicz A., Palewska K., Lipiński J., Kowal R., Swedek B.: *On the spectroscopic and nonlinear optical properties of 3-(1,1-dicyanoethenyl)-1-phenyl-4,5-dihydro-1H-pyrazole (DCNP)*. *Molecular Crystals and Liquid Crystals Science and Technology A*. 1994, Vol. 253, s. 41–50.
9. Nešpůrek S., Sworakowski J.: *Electroactive and photochromic molecular materials for wires, switches and memories*. *IEEE Engineering in Medicine and Biology Magazine*. 1994, Vol. 13, No. 1, s. 45–57.
10. Rohleder K., Luty T., Kuchta B.: *Orientational disorder modeling in mixed-stack molecular crystals*. *Journal of Chemical Physics*. 1994, Vol. 100, No. 2, s. 1573–1577.
11. Roszak S., Balasubramanian K.: *Organometallic analogues of the Diels–Alder reaction: molybdenum dimer + ethylene; molybdenum dimer + butadiene*. *Inorganic Chemistry*. 1994, Vol. 33, No. 18, s. 4169–4172.
12. Roszak S., Balasubramanian K.: *Reaction of the copper dimer with ethylene. A theoretical study*. *Chemical Physics Letters*. 1994, Vol. 231, No. 1, s. 18–24.
13. Roszak S., Balasubramanian K.: *Unresolved mathematical problems in the representation of potential energy surfaces by many-body potentials*. *Journal of Mathematical Chemistry*. 1994, Vol. 16, No. 1/2, s. 217–220.

14. Roszak S., Kaufman J.J., Koski W.S., Vijayakumar M., Balasubramanian K.: *Potential energy curves of ground and excited states of tetrahalomethanes and the negative ions*. Journal of Chemical Physics. 1994, Vol. 101, No. 4, s. 2978–2985.
15. Roszak S., Lowrey A.H., Sokalski A., Kaufman J.J.: *Usefulness of one electron properties in the study of the nitromethane-to-methyl nitrite rearrangement*. Journal of Molecular Graphics. 1994, Vol. 12, No. 3, s. 207–211.
16. Roszak S.: *A theoretical study of  $NO^{(-)}$  complexes with neutral water solvent molecules*. Chemical Physics Letters. 1994, Vol. 221, No. 3/4, s. 255–258.
17. Roszak S.: *A theoretical study of the  $N,N$ -dimethylnitramine structure*. Journal of Molecular Structure. Theochem. 1994, Vol. 110, No. 3, s. 269–272.
18. Sokalski A.: *Libraries of atomic multipole moments for precise modeling of electrostatic properties of amino acids*. Aminosan. 1994, Vol. 7, No. 1, s. 19–26.
19. Strasburger K., Sokalski A.: *Intramolecular electrostatic interactions studied by cumulative atomic multipole moment expansion with improved convergence*. Chemical Physics Letters. 1994, Vol. 221, No. 1/2, s. 129–135.
20. Sworakowski J., Palewska K., Bertault M.: *A calorimetric study of phase transitions in  $C_{70}$ fullerene*. Chemical Physics Letters. 1994, Vol. 220, No. 3–5, s. 197–202.
21. Sworakowski J., Palewska K., Bertault M.: *Phase transition in a  $C_{70}$ -toluene adduct*. Synthetic Metals. 1994, Vol. 64, No. 2/3, s. 323–327.
22. Sworakowski J.: *Effect of dipolar defects on trapping of charge carriers in highly anisotropic polydiacetylene crystals*. Molecular Crystals and Liquid Crystals Science and Technology A. 1994, Vol. 253, s. 233–242.
23. Szostak M.M., Le Calve N., Romain F., Pasquier B.: *LO-TO splittings, effective charges and interactions in electro-optic meta-nitroaniline crystal as studied by polarized IR reflection and transmission spectra*. Chemical Physics. 1994, Vol. 187, No. 3, s. 373–380.
24. Walton D.J., Phull S.S., Colton D., Richards P., Chyla A., Javed T., Clarke L., Lorimer J.P., Mason T.J.: *Ultrasonic enhancement of electrochemiluminescence from arylacetate electrooxidation*. Ultrasonics Sonochemistry. 1994, Vol. 1, No. 1, s. S23–S26.
25. Zboński Z., Styrz S.: *Predimeric pairs as traps for charge carriers in organic solids: Naphthalene and anthracene crystals*. Chemical Physics. 1994, Vol. 180, No. 1, s. 71–76.