

SCIGRESS Publications

- **A. Abdel-Karim, H. Elhaes, A.S. El-Kalliny**
Probing protein rejection behavior of blended PES-based flat-sheet ultrafiltration membranes: A density functional theory (DFT) study
Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy (2020) 238, 118399
- **Y.M. Issa, G. Abdel-Maksoud, M. Ibrahim**
A combination of analytical methods to evaluate the effect of humidity aging on the painting materials of icon models
Vibrational Spectroscopy (2020) 107, 103010
- **A.M. Bayoumy, A. Refaat, I.S. Yahia, H.Y. Zahran**
Functionalization of graphene quantum dots (GQDs) with chitosan biopolymer for biophysical applications
Optical and Quantum Electronics (2020) 52 (16)
- **E.M. Mamontova, A.L. Zakharenko, O.D. Zakharova**
Identification of novel inhibitors for the tyrosyl-DNA-phosphodiesterase 1 (Tdp1) mutant SCAN1 using virtual screening
Bioorganic & Medicinal Chemistry (2020) 28 (1), 115234
- **J.F. Fabre, G.N.M. Boussambe, R. Valentin, Z. Mouloungui**
Theoretical and Kinetic Analysis of the Esterification of Undecylenic Acid with Glycerol
Lipids (2020) 55 (4), 329-339
- **H.A. Ezzat, I. Gomaa, A.E.D.A. Gawad, O. Osman**
Semiempirical Molecular Modeling Analyses for Graphene/Nickel Oxide Nanocomposite
Letters in Applied NanoBioScience (2020) 9 (4), 1459 – 1466
- **S.P. Lakshmi, A.T. Reddy, L.D. Kodihela**
The tea catechin epigallocatechin gallate inhibits NF- κ B-mediated transcriptional activation by covalent modification
Archives of Biochemistry and Biophysics (2020) 695, 108620
- **N. Ornnork, D. Kiriwan, K. Lirdprapamongkol**
Molecular dynamics, MM/PBSA and in vitro validation of a novel quinazoline-based EGFR tyrosine kinase inhibitor identified using structure-based in silico screening
Journal of Molecular Graphics and Modelling (2020) 99, 107639
- **A.A. Elfiky**
Anti-HCV, nucleotide inhibitors, repurposing against COVID-19
Life Sciences (2020) 248, 117565
- **L. Perekhoda, V. Georgiyants, H. Yeromina, I. Drapak**
The Synthesis and In Silico Antihypertensive Activity Prognosis of New Mannich Bases Containing the 1, 2, 4-Triazole Moiety
Chem. Chem. Technol. (2020) 14 (2), 214–220
- **A.A. Elfiky**
SARS-CoV-2 RNA dependent RNA polymerase (RdRp) targeting: an in silico perspective
Journal of Biomolecular Structure and Dynamics (2020) 38, 1538-0254
- **A. A. Elfiky**
Ribavirin, Remdesivir, Sofosbuvir, Galidesivir, and Tenofovir against SARS-CoV-2 RNA dependent RNA polymerase (RdRp): A molecular docking study

- Life sciences (2020) 253, 117592*
- **Z. Piao, L. Zhu, X. Wang, P. Xiao, J. Zhou, B. Wang**
Effect of BaO on the viscosity and structure of fluorine-free calcium silicate-based mold flux
Journal of Non-Crystalline Solids (2020) 542, 120111
 - **H. Xiao, Y. Wang, X. Jia, L. Yang, X. Wang, X. Guo**
Tris (4-hydroxyphenyl) ethane (THPE), a trisphenol compound, is antiestrogenic and can retard uterine development in CD-1 mice
Environmental Pollution (2020) 260, 113962
 - **E.A. Mohamad**
In Silico Study of Ginger Extract and Capsaicin Effects on Prostate Cancer
Romanian Journal of Biophysics (2019) 29 (3), 81–87
 - **A.A. Elfiky, A. Ismail**
Molecular dynamics and docking reveal the potency of novel GTP derivatives against RNA dependent RNA polymerase of genotype 4a HCV
Life Sciences (2019) 238, 116958
 - **A.A. Elfiky**
The antiviral Sofosbuvir against mucormycosis: an in silico perspective
Future Virology (2019) 14(14), 739–744
 - **W.M. El Kayal, S.Y. Shtrygol, S.V. Zalevskyi**
Synthesis, in vivo and in silico anticonvulsant activity studies of new derivatives of 2-(2, 4-dioxo-1, 4-dihydroquinazolin-3 (2H)-yl) acetamide
European Journal of Medicinal Chemistry (2019) 180, 134-142
 - **A. Kolbus, A. Danel, D. Grabka, M. Kucharek**
Spectral Properties of Highly Emissive Derivative of Coumarin with N,N-Diethylamino, Nitrile and Thiophenecarbonyl Moieties in Water-Methanol Mixture
Journal of Fluorescence (2019) 29, 1393–1399
 - **Ł. Kaczmarek, T. Warga, P. Zawadzki, M. Makowicz, B. Bucholc, P. Kula**
The influence of the hydrogenation degree on selected properties of graphene as a material for reversible H₂ storage
International Journal of Hydrogen Energy (2019) 44 (41), 23149-23159
 - **K. Jedynak, B. Szczepanik, N. Rędzia, P. Słomkiewicz**
Ordered Mesoporous Carbons for Adsorption of Paracetamol and Non-Steroidal Anti-Inflammatory Drugs: Ibuprofen and Naproxen from Aqueous Solutions
Water (2019,)11 (5), 1099
 - **P. Chanphai, V. Ouellette, S. Mandal**
Location of multiple binding sites for testo and testo–Pt(II) with tRNA
Journal of Biomolecular Structure and Dynamics (2019) 37 (16)
 - **M.A. Revuelta-Maza, S. Nonell, G. De La Torre**
Boosting the singlet oxygen photosensitization abilities of Zn(ii) phthalocyanines through functionalization with bulky fluorinated substituents
Organic & Biomolecular Chemistry (2019) 32
 - **SP Lakshmi, AT Reddy, A Banno**
Molecular, chemical, and structural characterization of prostaglandin A₂ as a novel agonist for Nur77
Biochem J (2019) 476 (19): 2757–2767
 - **A. Vergara-Jaque, M. Zuniga, H. Poblete**
Computational Methodologies for Exploring Nano-engineered Materials
Nanoengineering Materials for Biomedical (2019) 57-79

- **O.W. Mak, R. Chand, J. Reynisson**
 Identification of Isoform-Selective Ligands for the Middle Domain of Heat Shock Protein 90 (Hsp90)
International Journal of Molecular Sciences (2019) 20 (21), 5333
- **R.S. Holt, T.R. Rybolt**
 Modeling Enhanced Adsorption of Explosive Molecules on a Hydroxylated Graphene Pore Graphene (2019) 8(1)
- **E. Mozhaitsev, E. Suslov, Y. Demidova**
 The Development of Tyrosyl-DNA Phosphodiesterase 1 (TDP1) Inhibitors Based on the Amines Combining Aromatic/Heteroaromatic and Monoterpenoid Moieties
Letters in Drug Design & Discovery (2019) 16(5), 597-605(9)
- **Y. Chen, M. Wang, H. Fu, X. Qu, Z. Zhang, F. Kang, D. Zhu**
 Spectroscopic and molecular modeling investigation on inhibition effect of nitroaromatic compounds on acetylcholinesterase activity
Chemosphere (2019) 236, 124365
- **D. Wiczew, A. Borowska, K. Szkaradek, T. Biegus**
 Molecular mechanism of vSGLT inhibition by gneyulin reveals antiseptic properties against multidrug-resistant gram-negative bacteria
Journal of Molecular Modeling (2019) 25 (186)
- **A. Hara, H. Kazimierzak, A. Bigos**
 Effect of Different Organic Additives on Surface Morphology and Microstructure of Zn-Mo Coatings Electrodeposited from Citrate Baths
Archives of Metallurgy and Materials (2019) 64 (1), 207-220
- **L.T. Tran, V. Blay, S. Luang, C. Eurtivong, S. Choknud**
 Engineering faster transglycosidases and their acceptor specificity
Green Chemistry (2019) 21, 2823-2836
- **M. Vonesch, J.A. Wytko, H. Kitagishi, K. Kano**
 Modelling haemoproteins: porphyrins and cyclodextrins as sources of inspiration
Chem. Commun., (2019) 55, 14558-14565
- **G. Basuyaux, A. Desmarchelier, G. Gontard**
 Extra hydrogen bonding interactions by peripheral indole groups stabilize benzene-1,3,5-tricarboxamide helical assemblies
Chemical Communications (2019) 55, 8548-8551
- **A. Hara, Z. Świątek, P. Ozga**
 The role of surfactants in induced electrodeposition of Zn–Mo layer from citrate solutions
Journal of Alloys and Compounds (2020) 827, 154195
- **K. Pyta, A. Janas, M. Szukowska, P. Pecyna**
 Synthesis, docking and antibacterial studies of more potent amine and hydrazone rifampicin congeners than rifampicin
European Journal of Medicinal Chemistry (2019) 167, 96-104
- **M. Pytlarczyk, P. Kula**
 Synthesis and mesomorphic properties of 4,4''-dialkynyl-2',3'-difluoro-p-terphenyls – the influence of C≡C acetylene linking bridge
Liquid Crystals (2019) 46 (4), 618-628
- **L. Escobar, P. Ballester**
 Quantification of the hydrophobic effect using water-soluble super aryl-extended calix[4]pyrroles
Organic Chemistry Frontiers (2019) 6, 1738-1748

- **C. Eurtivong, J. Reynisson**
 The Development of a Weighted Index to Optimise Compound Libraries for High Throughput Screening
Molecular Informatics (2019) 38 (3)
- **Ezat, A.A., Elfiky, A.A., Elshemey, W.M. et al.**
 Novel inhibitors against wild-type and mutated HCV NS3 serine protease: an in silico study
VirusDis. (2019) pp 1–7
- **Elfiky, Abdo A.**
 Novel Guanosine Derivatives as Anti-HCV NS5b Polymerase: A QSAR and Molecular Docking Study
Medicinal Chemistry (2019) 15,130-137(8)
- **Paneth, W. Płonka, P. Paneth**
 Assessment of Nonnucleoside Inhibitors Binding to HIV-1 Reverse Transcriptase Using HYDE Scoring
Pharmaceuticals (2019) 12(2), 64
- **E. Mozhaitsev, E. Suslov, Y. Demidova, D. Korchagina, K. Volcho, A. Zakharenko, I. Vasil'eva, M. Kupryushkin, A. Chepanova, D. Moscoh Ayine-Tora, J. Reynisson, N. Salakhutdinov, O. Lavrik**
 The Development of Tyrosyl-DNA Phosphodiesterase 1 (TDP1) Inhibitors Based on the Amines Combining Aromatic/Heteroaromatic and Monoterpenoid Moieties
Letters in Drug Design & Discovery (2019) 16, 597
- **C. Eurtivong, J. Reynisson**
 The Development of a Weighted Index to Optimise Compound Libraries for High Throughput Screening
Molecular informatics (2019) 38, 3
- **D. L. Wong, N. C. Korkolaa, M. J. Stillman**
 Kinetics of competitive Cd²⁺ binding pathways: the realistic structure of intrinsically disordered, partially metallated metallothioneins
Metallomics (2019) Advance Article
- **L. Escobar, P. Ballester**
 Quantification of the hydrophobic effect using water-soluble super aryl-extended calix[4]pyrroles
Org. Chem. Front. (2019) Advance Article
- **Hara, H. Kazimierczak, A. Bigos, Z. Świątek, P. Ozga**
 Effect of Different Organic Additives on Surface Morphology and Microstructure of Zn-Mo Coatings Electrodeposited from Citrate Baths
Arch. Metall. Mater. (2019) 64 (1), 207-220
- **Ashraf, F. Aman, S. Movassaghi, A. Zafar, M. Kubanik, W. A. Siddiqui, J. Reynisson, T. Söhnel, S. M. F. Jamieson, M. Hanif, C. G. Hartinger**
 Structural Modifications of the Antiinflammatory Oxicam Scaffold and Preparation of Anticancer Organometallic Compounds
Organometallics (2019) 38 (2), 361–374
- **Ahmed A. Ezat, Wael M. Elshemey**
 A comparative study of the efficiency of HCV NS3/4A protease drugs against different HCV genotypes using in silico approaches
Life Sciences (2019) 217, 176-184
- **S. Świątek, P. Komorek, G. Turner, B. Jachimiska**
 β-Lactoglobulin as a potential carrier for bioactive molecules

- Bioelectrochemistry (2019) 126, 137-145*
- **C. W. Frye, T. R. Rybolt**
Nanohashtag structures based on carbon nanotubes and molecular linkers
Surface Science (2018) 669, 34-44
 - **Angel Zhang, Martin J. Stillman**
Exploring function activated chlorins using MCD spectroscopy and DFT methods: design of a chlorin with a remarkably intense, red Q band
Phys. Chem. Chem. Phys. (2018) 20, 12470-12482
 - **Mahmoud, El-Sayed; Omar, Amina; Bayoumy, Ahmed M.; Ibrahim, Medhat**
Chitosan Ibuprofen Interaction: Modeling Approach
Sensor Letters (2018) 16, 347-355
 - **M. Makowicz, M. Balik, Ł. Kaczmarek, T. Warga, M. Stegliński, H. McPhillips, P. Kula**
Spatial functionalization of graphene powder using 1,4-dichlorobutane on ceramic substrate
Materials Chemistry and Physics (2018) 215, 376-384
 - **Edmundo G. Percástegui, Carlos Reyes-Mata, Marcos Flores-Alamo, Beatriz Quiroz-García, Ernesto Rivera, Ivan Castillo**
Transformations in Chemically Responsive Copper-Calixarene Architectures
Chemistry - An Asian Journal (2018) 13, 520-527
 - **Matteo Granelli Alan M. Downward, Claire Deville, Alejandro Rodriguez Franco, Laure Guénée, Céline Besnard, Alan F. Williams**
Coordination Chemistry of the Chiral, Facially Coordinating Tridentate Ligand 1,2-Bis(benzimidazol-2-yl)ethanol with 3d Transition Metals
European Journal of Inorganic Chemistry (2018) 37, 4181-4189
 - **Maciej Krzywiecki, Lucyna Grządziel, Paulina Powroźnik, Monika Kwoka, Julian Rechmann, Andreas Erbe**
Oxide-organic heterostructures: a case study of charge transfer disturbance at a SnO₂-copper phthalocyanine buried interface
Phys. Chem. Chem. Phys. (2018) 20, 16092-16101
 - **Rasha A. Youness, Mohammed A. Taha, Medhat Ibrahim**
In vitro bioactivity, physical and mechanical properties of carbonated-fluoroapatite during mechanochemical synthesis
Ceramics International (2018) 44, 21323-21329
 - **Ettore Fazio, Cally J. E. Haynes, Gema de la Torre, Jonathan R. Nitschke, Tomás Torres**
A giant M₂L₃ metallo-organic helicate based on phthalocyanines as a host for electroactive molecules
Chem. Commun. (2018) 54, 2651-2654
 - **L. Escobar, A. Díaz-Moscoso, P. Ballester**
Conformational selectivity and high-affinity binding in the complexation of N-phenyl amides in water by a phenyl extended calix[4]pyrrole
Chem. Sci. (2018) 9, 7186-7192
 - **Gordon W. Irvine, Natalie Korkola, Martin J. Stillman**
Isolated domains of recombinant human apo-metallothionein 1A are folded at neutral pH: a denaturant and heat-induced unfolding study using ESI-MS
Bioscience Reports (2018) 38, (4)
 - **Bożena Pietrzyk, Sebastian Miszczak, Łukasz Kaczmarek, Marek Klichxxx**

Low friction nanocomposite aluminum oxide/MoS₂ coatings prepared by sol-gel method
Ceramics International (2018) 44, 8534-8539

- **Paulina Powroźnik, Lucyna Grządziel, Wiesław J. Jakubik, Maciej Krzywiecki**
Sarin-simulant detection by phthalocyanine/palladium structures: From modeling to real sensor response
Sensors and Actuators B: Chemical (2018) 273, 771-777
- **Thomas R. Rybolt, Claire B. Black**
Polycyclic Aromatic Hydrocarbon Molecule-Surface Binding Energies in Site Specific Graphene Bilayer Nanopores: A Puzzle-ene Force Field Calculation
Graphene (2017) 6, 72-84
- **Marcin Kwit, Natalia Prusinowska, Robert Cysewski, Beata Warzajtis, Urszula Rychlewska, Jacek Gawroński**
A circular dichroism-DFT method for conformational study of flexible molecules: the case of 1- and 2-naphthyl diesters
Arkivoc (2017) part ii, 492-506
- **Akira Akaishi, Tomohiro Yonemaru, Jun Nakamura**
Formation of Water Layers on Graphene Surfaces
ACS Omega (2017) 2, 2184-2190
- **Vladimir Kubyshkin and Nediljko Budisa**
Construction of a polyproline structure with hydrophobic exterior using octahydroindole-2-carboxylic acid
Org. Biomol. Chem., 2017, 15, 619-627
- **Agata Paneth, Wojciech Płonka and Piotr Paneth**
What do docking and QSAR tell us about the design of HIV-1 reverse transcriptase nonnucleoside inhibitors?
J Mol Model (2017) 23: 317
- **Vladimir Kubyshkin and Nediljko Budisa**
Amide rotation trajectories probed by symmetry
Org. Biomol. Chem., 2017, 15, 6764-6772
- **Kamezaki C., Nakashima A., Yamada A., Uenishi S., Ishibashi H., Shibuya N., Hama S., Hosoi S., Yamashita E., Kogure K.**
Synergistic antioxidative effect of astaxanthin and tocotrienol by co-encapsulated in liposomes
J Clin Biochem Nutr (2016) Sep;59(2):100-106
- **M. Klein, R. Pankiewicz, M. Zalas, W. Stampor**
Magnetic field effects in dye-sensitized solar cells controlled by different cell architecture
Scientific Reports (2016) 6: 30077
- **Yosuke Kataoka**
Molecular Dynamics Simulations of Charge-Stabilized Colloidal Dispersions using the Sogami-Ise Potential
Int. J. Microgravity Sci. Appl. (2016) 33 (3) 330308
- **A. L. Bugaev, A. A. Guda, O. M. Yefanov, U. Lorenz, A. V. Soldatov, I. A. Vartanyants**
X-ray Absorption Spectroscopy and Coherent X-ray Diffraction Imaging for Time-Resolved Investigation of the Biological Complexes: Computer Modelling towards the XFEL Experiment
J. Phys.: Conf. Ser. (2016) 712 012024

- **Ken Albrecht, Yuki Hirabayashi, Masaya Otake, Shin Mendori, Yuta Tobari, Yasuo Azuma, Yutaka Majima, Kimihisa Yamamoto**
 Polymerization of a divalent/tetravalent metal-storing atom-mimicking dendrimer
Sci. Adv. (2016) 2: e1601414
- **Lina Perekhoda, Idibeg Kadamov, Narzullo Saidov, Victoriya Georgiyants**
 Synthesis of novel substituted 4-phenyl-5-phenoxyethyl-3-mercapto-1,2,4-triazole (4 H) derivatives as potential anti-ulcer agents
Scripta Scientifica Pharmaceutica (2015) vol. 2, No. 2, pp. 46-52
- **D. Hernández-Alonso, S. Zankowski, L. Adriaenssens, P. Ballester**
 Water-soluble aryl-extended calix[4]pyrroles with unperturbed aromatic cavities: synthesis and binding studies
Org. Biomol. Chem. (2015) 13, 1022
- **Shigeki Matsunaga**
 Effect of Greenhouse Gases Dissolved in Seawater
Int. J. Mol. Sci. (2015) 17, 45
- **Rakesh Kumar, Sangeeta Obrai, V K Joshi, Vikas Kumar, Siyamak Shahab**
 Computational, crystal structure and antimicrobial studies of directly synthesized dichloroethylenediaminecopper (II) complex
Commun. Inorg. Synth. (2015) Vol. 3, N°1, 9-15
- **Noha A. Saleh, Hanan Elhaes, Osama Osman, Abdel Aziz Mahmoud, Medhat Ibrahim**
 Spectroscopic Analyses of Modified Fulleropyrrolidine Derivatives
The Open Spectroscopy Journal (2015) 9, 1-6
- **Zarrag Al-Fifi, Noha A. Saleh, Hanan Elhaes, Medhat Ibrahim**
 On the Molecular Modeling Analyses of Novel HIV-1 Protease Inhibitors Based on Modified Chitosan Dimer
International Journal of Spectroscopy (2015), Article ID 174098, 9 pages
- **Elise M. Naughton, Mingqiang Zhang, Diego Troya, Karen J. Brewer, Robert B. Moore**
 Size dependent ion-exchange of large mixedmetal complexes into Nafion® membranes
Polym. Chem. (2015) 6, 6870
- **Natalia Prusinowska, Wioletta Bendzińska-Berus, Joanna Szymkowiak, Beata Warżajtis, Jadwiga Gajewy, Maciej Jelecki, Urszula Rychlewska, Marcin Kwit**
 Double helicity induction in chiral bis(triphenylacetamides)
RSC Adv. (2015) 5, 83448-83458
- **Toshihiko Hanai**
 In silico Modeling Study on Molecular Interactions in Reversed-Phase Liquid Chromatography
Journal of Chromatographic Science (2015) 53:1084–1091
- **Itoh H, Maeda H, Yamada S, Hori Y, Mino T, Sakamoto M.**
 BINOL-Al catalysed asymmetric cyclization and amplification: preparation of optically active menthol analogs
Org Biomol Chem (2015) 28;13(20):5817-25
- **Homayon J. Arabshahi, Michelle Van Rensburg, Lisa I. Pilkington, Chae Yeon Jeon, Mirae Song, Ling Mey Gridel, Euphemia Leung, David Barker, Milena Vuica-Ross, Konstantin P. Volcho, Alexandra L. Zakharenko, Olga I. Lavrik, Jóhannes Reynisson**
 A synthesis, in silico, in vitro and in vivo study of thieno[2,3-b]pyridine anticancer analogues
MedChemComm (2015) 6(11), 1987-1997

- **LIU Yang-Hua, ZHOU Zhi-Xiang, ZHANG Xiao-Long, LI Han-Dong**
Development of QSAR Model for Predicting the Mutagenicity of Aromatic Compounds
Chinese J. Struct. Chem. (2015) Vol. 34, No. 3, 324-334
- **Medhat Ibrahim, Osama Osman, Abdel aziz Mahmoud, Hanan Elhaes**
Spectroscopic analyses of water hyacinth: FTIR and modeling approaches
Der Pharma Chemica (2015) 7(9):182-188
- **A. V. Glushchenko, L. A. Perekhoda, V. A. Georgiyants**
Docking studies of the chemical components of the composition of *Bupleurum aureum* plant in relation to hepatoprotective biotargets
Der Pharma Chemica (2015) 7(4):201-206
- **Esteve-Turrillas FA, Mercader JV, Parra J, Agulló C, Abad-Somovilla A, Abad-Fuentes A**
Ready Access to Proquinazid Haptens via Cross-Coupling Chemistry for Antibody Generation and Immunoassay Development
PLoS One. (2015) 27;10(7): e0134042
- **Yoko Matsuura, Shuichi Arakawa, Masami Okamoto**
Single-stranded DNA adsorption characteristics by hollow spherule allophane nano-particles: pH dependence and computer simulation
Applied Clay Science (2014) 101, 591–597
- **Kulwinder Singh, Monika, Neelam Verma**
3-Dimensional QSAR and molecular docking studies of a series of indole analogues as inhibitors of human non-pancreatic secretory phospholipase A₂
Int J Res Med Sci. (2014) Aug;2(3):995-1002
- **Hamdy I.A. Mostafa, Nihal. S. El-bialy, Ahmed A. Ezat, Noha. A. Saleh, Medhat A. Ibrahim**
QSAR Analysis and Molecular Docking Simulation of Suggested Peptidomimetic NS3 Protease Inhibitors
Curr Comput Aided Drug Des. (2014) 10(1):28-40
- **Nohad A Al Omari, Mahmood H Jasim, Mohanad A Al Fahad**
In-silico Screening of Gold-Based Compounds as Potential Non Competitive Inhibitors for Human Mitochondrial Thioredoxin Reductase
AJADD (2014) 298-307
- **Boshkayeva Assyl, V. A. Georgiyants, L. O. Perekhoda**
Study of acyl substitution on docking properties of substituted dihydrogercetines as anti-inflammatory agents
Journal of Chemical and Pharmaceutical Research (2014) 6(4):749-753
- **Abdel Aziz Mahmoud, Osama Osman, Walid El-hotaby, Ahmed Fakhry, Zainab Abdel Aziz, Medhat Ibrahim, Hanan Elhaes**
Modeling and Molecular Spectroscopic Analyses of Cellulose
Journal of Applied Solution Chemistry and Modeling (2014) Volume 3, No. 3
- **ZHANG Xiao-Long, ZHOU Zhi-Xianga, LIU Yang-Huaa, FAN Xue-Lan, LI Han-Dong, WANG Jian-Tao**
Predicting the Acute Toxicity of Aromatic Amines by Linear and Nonlinear Regression Methods
Chinese J. Struct. Chem. (2014) Vol. 33, No. 2, 244–252
- **Kulwinder Singh, Monika, Neelam Verma**

3-Dimensional quantitative structure-activity relationship and molecular docking studies of tetrasubstituted pyrazole derivatives as inhibitors of cyclooxygenase-2

Int J Res Med Sci. (2014) May;2(2):612-619

- **Yuichi Sakanishi, Taisuke Arita, Mami Itoh, Takashi Saeki**
Rheological Properties and Self-Assembled Structures of Newly Synthesized Amide Organogelators, Butane 1,2,3,4-Tetracarboxamides, in Isododecane
Advances in Materials Physics and Chemistry (2014) 4, 267-274
- **Victoriya Georgiyants, Lina Perekhoda, Narzullo Saidov, Idibeg Kadamov**
Docking studies and biological evaluation of anti-cancer activity of new 1,2,4-triazole(4H) derivatives
Scripta Scientifica Pharmaceutica (2014) vol. 1, No. 2, pp. 46-53
- **Damien Simond, Sarah E. Clifford, Andreia F. Vieira, Céline Besnardb, Alan F. Williams**
An octahedral aluminium(III) complex as a three-fold node for supramolecular heterometallic self-assemblies: solution and solid state chemistry
RSC Adv. (2014) 4, 16686-16693
- **Subhasis Banerjee, Swastika Ganguly, Kalyan Kumar Sen, Kiattawee Choowongkomon, Supaporn Seetaha**
Synthesis, evaluation and binding mode analysis of some novel triazole derivatives as antimicrobials
Journal of Advanced Pharmacy Education & Research Oct-Dec (2013) Oct-Dec, Vol. 3, Issue 4
- **Akhilesh K. Yadav, Jayprakash Thakur, Om Prakash, Feroz Khan, Dharmendra Saikia, Madan M. Gupta**
Screening of flavonoids for antitubercular activity and their structure–activity relationships
Med Chem Res (2013) 22:2706-2716
- **Jae H. Son, Thomas R. Rybolt**
Force Field Based MM2 Molecule-Surface Binding Energies for Graphite and Graphene
Graphene (2013) 02. 18-34
- **Ahmed A. Fadda, Rasha E. El-Mekawy, Ahmed El-Shafei, Harold S. Freeman, David Hinks, Manal El-Fedawy**
Design, Synthesis, and Pharmacological Screening of Novel Porphyrin Derivatives
Journal of Chemistry (2013) Article ID 340230, 11 pages
- **Neal MD, Jia H, Eyer B, Good M, Guerriero CJ, Sodhi CP, Afrazi A, Prindle T Jr, Ma C, Branca M, Ozolek J, Brodsky JL, Wipf P, Hackam DJ**
Discovery and validation of a new class of small molecule Toll-like receptor 4 (TLR4) inhibitors
PLoS One. (2013) 12;8(6):e65779
- **Sergey Shityakov, Carola Förster**
Multidrug resistance protein P-gp interaction with nanoparticles (fullerenes and carbon nanotube) to assess their drug delivery potential: a theoretical molecular docking study
Int. J. Computational Biology and Drug Design (2013) Vol. 6, No. 4
- **Dharmendra Kumar Yadav, Feroz Khan, Arvind Singh Negi**
Pharmacophore modeling, molecular docking, QSAR, and in silico ADMET studies of gallic acid derivatives for immunomodulatory activity
J Mol Model (2012) 18:2513–2525

- **Kelly L. Summers a, AnjanPreet K. Mahrok b, Michael D.M. Dryden b, Martin J. Stillman**
Structural properties of metal-free apometallothioneins
Biochemical and Biophysical Research Communications 425 (2012) 485–492

- **Feroz Khan, Abha Meena, Ashok Sharma**
QSPR & Docking Based Virtual Screening of Anti-Cancer Leads
Biobytes, Volume 4, March 2009, Page 43-46
- **A. Altun, K. Golcuk, M. Kumru**
Vibrational and thermal studies of metal(II) [Ni(II), Zn(II) and Cd(II)] iodide m-methylaniline complexes
Vibrational Spectroscopy, Volume 31, Issue 2, 6 May 2003, Pages 215-225
- **A. Altun, K. Golcuk, M. Kumru**
Vibrational and thermal studies of p-methylaniline complexes with Ni(II), Zn(II) and Cd(II) iodides
Vibrational Spectroscopy, Volume 33, Issues 1-2, 19 December 2003, Pages 63-74
- **A. Huczynski, I. Binkowska, A. Jarczewski, B. Brzezinski**
Spectroscopic studies of the 1:1 complexes of 4-nitrophenyl[bis(ethylsulfonyl)]methane and phenyl[bis(ethylsulfonyl)]methane with 7-methyl-1,5,7-triazabicyclo[4.4.0]dec-5-ene and 1,5,7-triazabicyclo[4.4.0]dec-5-ene
Journal of Molecular Structure, Volume 841, Issues 1-3, 30 September 2007, Pages 133-136
- **Aakeroy, Christer B. and Peter B. Hitchcock and Kenneth R. Seddon.**
Organic Salts of L-Tartaric Acid: Materials for Second Harmonic Generation with a Crystal Structure Governed by an Anionic Hydrogen-Bonded Network.
J. Chem. Soc., Chem. Commun., 1992, pp. 553-555.
- **Adam Huczynski, Bogumil Brzezinski, Franz Bartl**
Structures of complexes of benzyl and allyl esters of monensin A with Mg²⁺, Ca²⁺, Sr²⁺, Ba²⁺ cations studied by ESI-MS and PM5 methods
Journal of Molecular Structure, In Press, Corrected Proof, Available online 1 November 2007
- **Adam Huczynski, Daniel Łowicki, Bogumil Brzezinski, Franz Bartl**
Spectroscopic, mass spectrometry and semiempirical investigation of a new 2-methoxyethyl ester of monensin A and its complexes with Li⁺, Na⁺ and K⁺ cations
Journal of Molecular Structure, Volume 874, Issues 1-3, 28 February 2008, Pages 89-100
- **Adam Huczynski, Daniel Łowicki, Bogumil Brzezinski, Franz Bartl**
Spectroscopic, mass spectrometry, and semiempirical investigations of a new 2-(2-methoxyethoxy)ethyl ester of Monensin A and its complexes with monovalent cations
Journal of Molecular Structure, Volume 879, Issues 1-3, 15 May 2008, Pages 14-24
- **Adam Huczynski, Dominik Michalak, Piotr Przybylski, Bogumil Brzezinski, Franz Bartl**
Monensin A benzyl ester and its complexes with monovalent metal cations studied by spectroscopic, mass spectrometry and semiempirical methods
Journal of Molecular Structure, Volume 797, Issues 1-3, 18 September 2006, Pages 99-110
- **Adam Huczynski, Dominik Michalak, Piotr Przybylski, Bogumil Brzezinski, Franz Bartl**
Spectroscopic, mass spectrometry and semiempirical investigation of a new Monensin A allyl ester and its complexes with Li⁺, Na⁺ and K⁺cations
Journal of Molecular Structure, Volume 828, Issues 1-3, 28 February 2007, Pages 130-141
- **Adam Huczynski, Małgorzata Ratajczak-Sitarz, Andrzej Katrusiak, Bogumil Brzezinski**
Molecular structure of rubidium six-coordinated dihydrate complex with monensin A
Journal of Molecular Structure, In Press, Corrected Proof, Available online 15 December 2007

- **Adam Huczynski, Małgorzata Ratajczak-Sitarz, Andrzej Katrusiak, Bogumil Brzezinski**
Molecular structure of the 1:1 inclusion complex of monensin A lithium salt with acetonitrile
Journal of Molecular Structure, Volume 871, Issues 1-3, 15 December 2007, Pages 92-97
- **Adam Huczynski, Małgorzata Ratajczak-Sitarz, Andrzej Katrusiak, Bogumil Brzezinski**
Molecular structure of the 1:1 inclusion complex of monensin A sodium salt with acetonitrile
Journal of Molecular Structure, Volume 832, Issues 1-3, 30 April 2007, Pages 84-89
- **Adam Huczynski, Piotr Przybylski, Bogumil Brzezinski**
NMR, FTIR, ESI-MS and semiempirical study of a new 2-(2-hydroxyethoxy)ethyl ester of monensin A and its complexes with alkali metal cations
Tetrahedron, Volume 63, Issue 36, 3 September 2007, Pages 8831-8839
- **Adam Huczynski, Piotr Przybylski, Bogumił Brzezinski**
Complexes of monensin A methyl ester with Mg²⁺, Ca²⁺, Sr²⁺, Ba²⁺ cations studied by electrospray ionization mass spectrometry and PM5 semiempirical method
Journal of Molecular Structure, Volume 788, Issues 1-3, 8 May 2006, Pages 176-183
- **Adam Huczynski, Piotr Przybylski, Grzegorz Schroeder, Bogumił Brzezinski**
Investigation of complex structures of a new 2-hydroxyethyl ester of Monensin A with Mg²⁺, Ca²⁺, Sr²⁺, Ba²⁺ cations using electrospray ionization mass spectrometry and semiempirical PM5 methods
Journal of Molecular Structure, Volume 829, Issues 1-3, 17 March 2007, Pages 111-119
- **Adam Huczynski, Rafał Wawrzyn, Bogumil Brzezinski, Franz Bartl**
Structure of complexes of lasalocid m-nitrobenzyl ester with monovalent metal cations
Journal of Molecular Structure, In Press, Corrected Proof, Available online 1 February 2008
- **Adam Huczynski, Tomasz Pospieszny, Małgorzata Ratajczak-Sitarz, Andrzej Katrusiak, Bogumil Brzezinski**
Structural and spectroscopic studies of the 1:1 complex of lasalocid acid with 1,5,7-triazabicyclo[4.4.0]dec-5-ene
Journal of Molecular Structure, Volume 875, Issues 1-3, 17 March 2008, Pages 501-508
- **Adam Huczynski, Tomasz Pospieszny, Rafał Wawrzyn, Małgorzata Ratajczak-Sitarz, Andrzej Katrusiak, Bogumil Brzezinski, Franz Bartl**
Structural and spectroscopic studies of new o-, m- and p-nitrobenzyl esters of lasalocid acid
Journal of Molecular Structure, Volume 877, Issues 1-3, 17 April 2008, Pages 105-114
- **Ahmet Altun, Kurtulus Golcuk, Mustafa Kumru, Abraham F. Jalbout**
Electron-conformational study for the structure–hallucinogenic activity relationships of phenylalkylamines
Bioorganic & Medicinal Chemistry, Volume 11, Issue 18, 1 September 2003, Pages 3861-3868
- **Amit Basak, Subhendu Sekhar Bag, Ajoy Basak**
Design and synthesis of a novel enediynyl pentapeptide with predominantly β -turn structural motif and its potential as a fluorescence-based chemosensor
Bioorganic & Medicinal Chemistry, Volume 13, Issue 12, 2 June 2005, Pages 4096-4102
- **Andreas Klamt**
References
COSMO-RS, 2005, Pages 221-229
- **Andreas Zogg, Ulrich Fischer, Konrad Hungerbühler**
Identification of kinetic and thermodynamic reaction parameters from online calorimetric and IR-ATR data using a new combined evaluation algorithm
Chemical Engineering Science, Volume 59, Issue 24, December 2004, Pages 5795-5806
- **Anna Drabczynska, Christa E. Müller, Anke Schiedel, Britta Schumacher, Janina Karolak-Wojciechowska, Andrzej Fruzinski, Weronika Zobnina, Olga Yuzlenko, Katarzyna Kieć-Kononowicz**

Phenylethyl-substituted pyrimido[2,1-f]purinediones and related compounds: Structure–activity relationships as adenosine A1 and A2A receptor ligands

Bioorganic & Medicinal Chemistry, Volume 15, Issue 22, 15 November 2007, Pages 6956–6974

- **Anna Drabczynska, Christa E. Müller, Svenja K. Lacher, Britta Schumacher, Janina Karolak-Wojciechowska, Antony Nasal, Piotr Kawczak, Olga Yuzlenko, Elżbieta Pękala, Katarzyna Kieć-Kononowicz**
Synthesis and biological activity of tricyclic arylimidazo-, pyrimido-, and diazepinopurinediones
Bioorganic & Medicinal Chemistry, Volume 14, Issue 21, 1 November 2006, Pages 7258–7281
- **Arjan W. Kleij, Robert A. Gossage, Robertus J. M. Klein Gebbink, Nils Brinkmann, Ed J. Reijerse, Udo Kragl, Martin Lutz, Anthony L. Spek, and Gerard van Koten**
A “Dendritic Effect” in Homogeneous Catalysis with Carbosilane-Supported Arylnickel(II) Catalysts: Observation of Active-Site Proximity Effects in Atom-Transfer Radical Addition
Journal of the American Chemical Society; 2000,122, 12112–12124.
- **Armin Sautter, Dietmar G. Schmid, Gunther Jung, and Frank Wurthner**
A Triangle-Square Equilibrium of Metallosupramolecular Assemblies Based on Pd(II) and Pt(II) Corners and Diazadibenzoperylene Bridging Ligands
Journal of the American Chemical Society; 2001,123, 5424–5430.
- **Astrid Netz, Kurt Polborn, and Thomas J. J. Muller**
Diastereoselective Propargylations with Planar Chiral Chromiumcarbonyl Arene Complex Substituted Propargyl Cations (Scientific Paper)
Journal of the American Chemical Society; 2001,123, 3441–3453.
- **Balkus, K.J., et al.**
Synthesis of aluminium phosphate molecular sieves using cobalticinium hydroxide.
Microporous Materials, No. 3, 1995 pp. 489–495.
- **Balkus, K.J., Krystyna Nowinska**
Intrazeolite organometallics Pentamethylcyclopentadienyl rhodium complexes.
Microporous Materials, No. 3, 1995, pp. 665–686.
- **Barry M. Trost and Hisanaka Ito**
A Direct Catalytic Enantioselective Aldol Reaction via a Novel Catalyst Design
Journal of the American Chemical Society; 2000,122, 12003–12004.
- **Berthold Kersting, Michel Meyer, Ryan E. Powers, and Kenneth N. Raymond**
Dinuclear Catecholate Helicates: Their Inversion Mechanism
J. Am. Chem. Soc. 1996, 118(30), 7221–7222.
- **Błażej Gierczyk, Grzegorz Schroeder, Piotr Przybylski, Bogumil Brzezinski, Franz Bartl, Georg Zundel**
ESI MS, NMR and PM5 semiempirical studies of oligomycin A and its complexes with Li⁺ and Na⁺ cations
Journal of Molecular Structure, Volume 738, Issues 1–3, 14 March 2005, Pages 261–270
- **Bodor, Nicholas, Huang, Ming-Ju**
On the Reactivity of CF_nH_{3–n}CHX (n=0,1,2, and 3, and X=H or Halogen atom)
Tetrahedron, Vol. 48, pp. 5823–5830, 1992.
- **Bodor, Nicholas, Huang, Ming-Ju**
Optimized structures and relative stabilities of the isomers of (CO₂)_{2n+1} (1<n
Chemical Physics Letters, Volume 192, number 4, 8 May 1992.
- **Bodor, Nicholas, Huang, Ming-Ju**
Predicting Partition Coefficients for Isomeric Diastereoisomers of Some Tripeptide Analogs
Journal of Computational Chemistry, Vol. 12, No. 10, 1182–1186, (1991).

- **Bodor, Nicholas, Huang, Ming-Ju,**
Intermolecular Interactions of Methyl Acetate, Beta-Propiolactone, Ethyl Acetate, and gamma-butyrolactone: an AM1 Semiempirical study.
International Journal of Quantum Chemistry, Vol. 44, 81-89 (1992).
- **Bodor, Nicholas, Huang, Ming-Ju, Kaminski, J.J.**
A theoretical study of prednisolone, 6(-fluoroprednisolone, 9(-fluoroprednisolone, 6(,9(-difluoroprednisolone and related compounds
Journal of Molecular Structure (Theochem), 279 (1993) 59-69.
- **Bodor, Nicholas, Kumar, Gondi, Huang, Ming-Ju, Hammer, Richard**
Soft Drugs. 17: Quantitative Structure-Activity Relationships of Soft Anticholinergics Based on Methatropine and Methscopolamine
Journal of Pharmaceutical Sciences, Vol. 83, No.1, January 1994.
- **Bogumił Brycki, Anna Sz wajca**
Spectroscopic characterization and single molecule structures of N,N-bis-(3-phthalimidopropyl)-N-(2-hydroxyethyl)-N-propylammonium salts and their hydrates
Journal of Molecular Structure, Volume 879, Issues 1-3, 15 May 2008, Pages 7-13
- **Bogusława Łęska, Grzegorz Schroeder, Teresa Łuczak, Piotr Przybylski, Radosław Pankiewicz, Maria Bełtowska-Brzezinska, Bogumił Brzezinski**
Structure and electrochemical reactivity of 3-[tris(2-methoxyethoxy)silyl]-propanethiol adsorbed on silver surface
Thin Solid Films, Volume 515, Issue 1, 25 September 2006, Pages 152-157
- **Bogusława Łęska, Piotr Przybylski, Joanna Wyrwał, Bogumił Brzezinski, Grzegorz Schroeder, Volodimir Rybachenko**
The reaction heats and PM5 semiempirical studies of complexes formed between silicon podand and Li⁺ cations
Journal of Molecular Structure, Volume 741, Issues 1-3, 2 May 2005, Pages 11-17
- **Bogusława Łęska, Piotr Przybylski, Joanna Wyrwał, Bogumił Brzezinski, Grzegorz Schroeder, Volodimir Rybachenko, Angelamaria Maia**
The reaction heats and PM5 semiempirical studies of complexes formed between silicon podand and monovalent cations
Journal of Molecular Structure, Volume 733, Issues 1-3, 3 January 2005, Pages 231-237
- **Bogusława Łęska, Radosław Pankiewicz, Grzegorz Schroeder, Angelamaria Maia**
Application of a new class B-podands in solid-liquid phase transfer catalysis
Journal of Molecular Catalysis A: Chemical, Volume 269, Issues 1-2, 18 May 2007, Pages 141-148
- **Bogusława Łęska, Radosław Pankiewicz, Grzegorz Schroeder, Błażej Gierczyk, Hieronim Maciejewski, Bogdan Marciniak**
New type of repeated Si-C-podand catalysts for solid-liquid phase transfer reactions
Catalysis Communications, Volume 9, Issue 5, 20 March 2008, Pages 821-825
- **Bogusława Łęska, Radosław Pankiewicz, Oksana Nevecheriya, Volodimir I. Rybachenko, Grzegorz Schroeder, Bogumił Brzezinski**
B-podand complexes with sodium ions: the reaction heats and PM5 semiempirical calculation
Journal of Molecular Structure, Volume 840, Issues 1-3, 17 September 2007, Pages 1-5
- **Bogusława Łęska, Iwona Kauna, Baej Gierczyk, Grzegorz Schroeder, Piotr Przybylski, Bogumił Brzezinski**
Kinetic studies of complexation reaction of polyoxaalkyl phosphates with Fe(III) in ethanol
Journal of Molecular Structure, Volume 643, Issues 1-3, 19 December 2002, Pages 9-19
- **Bottomley, Frank et al.**
Organometallic Oxides: Preparation and Properties of the Clusters (n-C₅Me₅)₄Mo₅O₁₁ and

$\{[(n-C_5Me_5)Mo]_3(n-OH)_n(n-O)_6-n\}C_{12}$.

J. Am. Chem. Soc., 116, 1994, pp. 7989-7995.

- **Brewster, Marcus E., et al.**
Application of Semiempirical Molecular Orbital Techniques to the Study of Peroxidase-Mediated Oxidation of Phenols, Anilines, Sulfides and Thiobenzamides.
Tetrahedron, Vol. 47, No. 36, 1991, pp. 7525-7536.
- **Brewster, Marcus E., et al.**
Reactivity of Biologically Important Reduced Pyridines. VIII. A Semiempirical (AM1) Study of the Oxidation of 3-Substituted-1-Methyl-1,4-Dihydropyridines.
Journal of Computational Chemistry, Vol. 12, No. 10, 1991, pp. 1278-1282.
- **Brewster, Marcus E., Huang, Ming-Ju, Bodor, Nicholas**
Reactivity of biologically important reduced pyridines. Part 9. Effect of substitution on rotational energetics in 1-phenyl-1,4-dihydropyridine, the 1-phenylpyridinium cation and related systems
Journal of Molecular Structure (Theochem), 257 (1992) 49-56.
- **Brewster, Marcus E., Huang, Ming-Ju, Pop, Emil, Bodor, Nicholas**
Hydroxyl Stretching in Substituted Phenols: an AM1 Study
International Journal of Quantum Chemistry, Quantum Biology Symposium 20, 7-15 (1993).
- **Brewster, Marcus E., Pop, Emil, Huang, Ming-Ju, Bodor, Nicholas**
Rotational barriers in phenol and sterically congested phenol derivatives, an AM1 study.
Journal of Molecular Structure (Theochem), 303 (1994) 25-38.
- **C. Luo, D. M. Guldi, H. Imahori, K. Tamaki, and Y. Sakata,**
Sequential Energy and Electron Transfer in an Artificial Reaction Center: Formation of a Long-Lived Charge-Separated State
Journal of the American Chemical Society; 2000,122, 6535-6551.
- **Carlos Bustos, Christian Sánchez, Rolando Martínez, Ricardo Ugarte, Eduardo Schott, Desmond Mac-Leod Carey, María Teresa Garland, Luis Espinoza**
Tautomeric, spectroscopic, DFT calculations and X-ray studies on O₂N-4-C₆H₄-NHN=C(COCH₃)₂
Dyes and Pigments, Volume 74, Issue 3, 2007, Pages 615-621
- **Carlota Conesa and Henry S. Rzepa**
PM3 and ab initio studies of the C₈ H₈ potential energy surface. Thermal isomerism of syn- and anti-tricyclo[4.2.0.0]octa-3,7-dienes
J. Chem. Soc., Perkin Trans. 2, 1998, 857.
- **Carlota Conesa and Henry S. Rzepa, Department of Chemistry,**
Re-engineering potential energy surfaces: trapezoidally distorted pi₂s + thermal cycloaddition/elimination reactions
J. Chem. Soc., Perkin Trans. 2, 1998, 269-2698.
- **Catalina E. Laplaza, Marc J. A. Johnson, Jonas C. Peters, Aaron L. Odom, Esther Kim, Christopher C. Cummins, Graham N. George, and Ingrid J. Pickering**
Dinitrogen Cleavage by Three-Coordinate Molybdenum(III) Complexes: Mechanistic and Structural Data 1
J. Am. Chem. Soc. 1996, 118(36), 8623-8638.
- **Chamot, Ernest, et al.**
Modeling Acid Sites in MFI Zeolites with Realistic Geometric Constraints.
Symposium on Molecular Modeling of Petroleum Processes and Catalysis, April 5-10, 1992.
- **Chamot, Ernest, et al.,**
Probing Polyolefin Stabilities by Semiempirical Methods.
Symposium on Industrial Applications of Quantum Chemistry, May 31-June 2, 1995.

- **Chien-Tien Chen and Y-Chen Chou,**
C₂-Symmetric Dibenzosuberane-Based Helicenes as Potential Chirochromic Optical Switches
Journal of the American Chemical Society; 2000,122, 7662-7672.
- **Chisako Yamagami, Miki Akamatsu, Noriko Motohashi, Shogo Hamada, Takao Tanahashi**
Quantitative structure–activity relationship studies for antioxidant hydroxybenzalacetones by quantum chemical- and 3-D-QSAR(CoMFA) analyses
Bioorganic & Medicinal Chemistry Letters, Volume 15, Issue 11, 2 June 2005, Pages 2845-2850
- **Christian Brückner, Michael A. Hyland, Ethan D. Sternberg, Jill K. MacAlpine, Steven J. Rettig, Brian O. Patrick, David Dolphin**
Preparation of [meso-tetraphenylchlorophinato]nickel(II) by stepwise deformylation of [meso-tetraphenyl-2,3-diformyl-secochlorinato]nickel(II): conformational consequences of breaking the structural integrity of nickel porphyrins
Inorganica Chimica Acta, Volume 358, Issue 10, 15 June 2005, Pages 2943-2953
- **Christodoulos Makedonas, Christiana A. Mitsopoulou**
A vibrational and DFT study of M(diimine)(dithiolate) complexes and their complexation route
Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, Volume 64, Issue 4, July 2006, Pages 918-930
- **Cikui Liang, David Gallagher**
Prediction of Physical and Chemical Properties by QSPR
American Laboratory, March 1997.
- **Colin J. Campbell, James F. Rusling, and Christian Brückner,**
Nickel(II) meso-Tetraphenyl-Homoporphyrins, -secochlorins, and -chlorophin: Control of Redox Chemistry by Macrocycle Rigidity
Journal of the American Chemical Society; 2000,122, 6679-6685.
- **Colin, Thomas, Gerad Bernardinelli, Charles W. Jefford, Djordje Maric and Jacques Weber**
Computational Studies of the Structures and Properties of Antimalarial Compounds Based on the 1,2,4-Trioxane Ring Structure. In Artemisinin-like Molecules.
International Journal of Quantum Chemistry, Vol. 21, 1991, pp. 117-131.
- **Colin, Thomas, Marshall Cory and Michael Zerner**
Theoretical Studies of Some New Anti-Malarial Drugs.
International Journal of Quantum Chemistry, 18, 1991, pp. 231-245.
- **Dana L. Caulder, Christian Bruckner, Ryan E. Powers, Stefan Konig, Tatjana N. Parac, Julie A. Leary, and Kenneth N. Raymond**
Design, Formation and Properties of Tetrahedral M₄L₄ and M₄L₆ Supramolecular Clusters
Journal of the American Chemical Society; 2001,123, 8923-8938.
- **Dani Youssef, Christie E. Nichols, T. Stanley Cameron, Jan Balzarini, Erik De Clercq, Amitabh Jha**
Design, synthesis, and cytostatic activity of novel cyclic curcumin analogues
Bioorganic & Medicinal Chemistry Letters, Volume 17, Issue 20, 15 October 2007, Pages 5624-5629
- **Davey, Simon N., Leigh, David A., Moody, Andrew E., Tetler, Lee W., Wade, Frances A.,**
C₆₀-Azacrown Ethers: the First Monoaminated Fullerene Derivatives
J. Chem. Soc. Chem. Commun., 1994.
- **David J. Edwards, Robin G. Pritchard, Timothy W. Wallace**
Complementary kinetic and thermodynamic resolution of a chiral biaryl axis
Tetrahedron Letters, Volume 44, Issue 25, 16 June 2003, Pages 4665-4668

- **De Paula, Julio C., Walters, Valerie A., et al.,**
Electronic Structure of Triplet States of Zinc(II) Tetraphenylporphyrins.
The Journal of Physical Chemistry, Vol. 99, No. 4, 1995, pp. 1166-1171.
- **DeShong, P. et al.**
A Novel Method for the Synthesis of Spiroketal Systems. Synthesis of the Pheromones of the Common Wasp and the Olive Fruit Fly.
J. Org. Chem., Vol. 56, 1991, 3207.
- **DeShong, P. et al.**
Improved Protocols for the Selective Deprotection of Trialkylsilyl Ethers Using Fluorosilicic Acid.
J. Org. Chem., 58, 1993, 5130.
- **DeShong, P. et al.**
Probing the Chemistry of Organomanganese Complexes. A Kinetic Study of the Demetalation of Manganacycles and Correlations of the Kinetic Parameters with Manganese-55 Chemical Shifts.
J. Org. Chem., Vol. 54, 1989, 5432.
- **DeShong, P. et al.**
Probing the Chemistry of Organomanganese Complexes. A Kinetic Study of the Role Coordinate Bonds in a Demetalation Reaction.
Tetrahedron, 1993, 5673.
- **DeShong, P. et al.**
Selective Deprotection of Trialkylsilyl Esters Using Fluorosilicic Acid.
J. Org. Chem., 56, 1991, 2492.
- **DeShong, P. et al.**
Synthesis of Tetramic Acid Antibiotics.
Studies in Natural Product Chemistry, Atta-Ur-Amman, Ed., Vol. 14, Elsevier: Amsterdam, 1993, pp. 97-142.
- **DeShong, P. et al.**
Total Synthesis of (+/-)-Tirandamycin B.
J. Am. Chem. Soc., 113, 1991, 8791.
- **DeShong, P. et al.**
Utilization of Tetrabutylammonium Triphenylsilyldifluoride (TBAT) as a Fluoride Source for Nucleophilic Fluorination.
J. Am. Chem. Soc., 117, 1995, 5166.
- **DeShong, P. et al., in "The Anomeric Effect and Associated Stereoelectronic Effects", Thatcher, G.**
Glycosylmanganese Complexes and Anomeric Anomalies. The Next Generation?
American Chemical Society: Washington D.C., ACS Series 539, 1993, pp. 227-238.
- **Douglass F. Taber, Kamfia K. You, and Arnold L. Rheingold**
Predicting the Diastereoselectivity of Rh-Mediated Intramolecular C-H Insertion
J. Am. Chem. Soc. 1996, 118(3), 547-556.
- **Douglass F. Taber, Wei Zhang, Carlton L. Campbell, Arnold L. Rheingold, and Christopher D. Incarvit**
Cyclozirconation of a Computationally-Designed Diene: Synthesis of (-)-Androst-4-ene-3,16-dione
Journal of the American Chemical Society; 2000,122, 4813-4814.
- **Doyle, Michael P., Westrum, Larry J., Wolthuis, Wendelmoed N.E., See, Marjorie M., Boone, William P., Bagheri, Vahid, Pearson, Matthew M.**
Electronic and Steric control in Carbon-Hydrogen Insertion Reactions of Diazoacetoacetates

Catalyzed by Dirhodium(II) Carboxylates and Carboxamides

J. Am. Chem. Soc., 115, 1993, pp. 958-964.

- **Doyle, Michael P., Westrum, Larry J., Wolthuis, Wendelmoed N.E., See, Marjorie M., Boone, William P., Bagheri, Vahid, Pearson, Matthew M.,**
Dirhodium (II) Tetrakis (carboxamidates) with Chiral Ligands. Structure and Selectivity in Catalytic Metal-Carbene Transformations.
Journal of the American Chemical Society, Vol. 115, No. 22, 1993, pp. 9968-9978.
- **F. Meinardi, M. Cerminara, S. Blumstengel, A. Sassella, A. Borghesi, and R. Tubino**
Broad and narrow bands in the photoluminescence spectrum of solid-state oligothiophenes: Two marks of an intrinsic emission
Phys. Rev. B 67, 184205 (2003)
- **F. Meinardi, S. Blumstengel, M. Cerminara, G. Macchi, and R. Tubino**
Intrinsic excitonic luminescence in crystalline terthiophene
Phys. Rev. B 72, 035207 (2005)
- **Frank Neese, Jeffrey M. Zaleski, Kelly Loeb Zaleski, and Edward I. Solomon**
Electronic Structure of Activated Bleomycin: Oxygen Intermediates in Heme versus Non-Heme Iron
Journal of the American Chemical Society; 2000,122(47), 11703-11724.
- **Frederick D. Lewis, Rajdeep S. Kalgutkar, and Jye-Shane Yang**
Highly Regioselective Anaerobic Photocyclization of 3-Styrylpyridines
Journal of the American Chemical Society; 2001,123, 3878-3884.
- **Fryzuk, Michael D., Haddad, T.S., Mylvaganam, Murugesapillai, McConville, David H., Rettig, Steven J.**
End-on Versus Side-On Bonding of Dinitrogen to Dinuclear Early Transition-Metal Complexes
J. Am. Chem. Soc., 115, 1993, pp. 2782-2792.
- **Fryzuk, Michael D., Xiaoliang Gao, and Steven J. Rettig,**
Reaction of the Coordinatively Unsaturated Methylene Complex $\text{Ir}=\text{CH}_2[\text{N}(\text{SiMe}_2\text{CH}_2\text{PPh}_2)_2]$ with Olefins: Stereoselective Formation of Allyl Hydride Derivatives
J. Am. Chem. Soc. 1995, 117, 3106-3117.
- **Fujita, Makoto, Satoshi Nagao, Katsuyuki Ogura,**
Guest-Induced Organization of a Three- Dimensional Palladium(II) Cagelike Complex. A Prototype for Induced-Fit Molecular Recognition
J. Am. Chem. Soc. 1995, 117, 1649-1650.
- **Gabrielov, A.G., K.J. Balkus, Jr., S.L. Bell, F. Bedioui, J. Devynck**
Faujasite zeolites modified with iron perfluorophthalocyanines: synthesis and characterization.
Microporous Materials, No. 2, 1994, pp.119-226.
- **Gallagher DA.**
Thermal Degradation of Nylon
Sci. Comp. Auto. Jun 1996.
- **George Domazetis, Monthida Raoarun, Bruce D. James, John Liesegang**
Molecular modelling and experimental studies on steam gasification of low-rank coals catalysed by iron species
Applied Catalysis A: General, Volume 340, Issue 1, 15 May 2008, Pages 105-118
- **Gheorghe Surpateanu, Paul Ionut Dron, David Landy, Sophie Fourmentin, Marc Bria**
Synthesis, inclusion capabilities, and electrical properties of some asymmetrical cyclophanes
Tetrahedron, Volume 64, Issue 4, 21 January 2008, Pages 721-732

- **Gina M. Stewart and Marye Anne Fox**
Chromophore-Labeled Dendrons as Light Harvesting Antennae
J. Am. Chem. Soc. 1996, 118(18), 4354-4360.
- **Grzegorz Bejcar, Piotr Przybylski, Bogumil Brzezinski**
NMR, FT-IR as well as PM5 semiempirical studies of new hydrazone of gossypol with 3-oxa-n-butylhydrazine
Journal of Molecular Structure, Volume 734, Issues 1-3, 31 January 2005, Pages 45-49
- **Grzegorz Bejcar, Piotr Przybylski, Joanna Fusiara, Bogumil Brzezinski, Franz Bartl**
1H, 13C NMR, FT-IR as well as PM5 semiempirical studies of new hydrazone of gossypol with 2,2?-diethoxyethyl hydrazine
Journal of Molecular Structure, Volume 743, Issues 1-3, 31 May 2005, Pages 145-149
- **Grzegorz Bejcar, Piotr Przybylski, Joanna Fusiara, Bogumil Brzezinski, Franz Bartl**
Spectroscopic and PM5 semiempirical studies of new hydrazone of gossypol with 3,6-dioxaheptylhydrazine
Journal of Molecular Structure, Volume 754, Issues 1-3, 8 November 2005, Pages 31-36
- **Grzegorz Bejcar, Piotr Przybylski, Monika Walkowiak, Bogumil Brzezinski**
Spectroscopic studies and PM5 semiempirical calculations of new hydrazone of gossypol with 3,6,9-trioxadecylhydrazine
Journal of Molecular Structure, Volume 830, Issues 1-3, 30 March 2007, Pages 72-77
- **Grzegorz Schroeder, Jaromir Kira, Tadeusz Ossowski, Bogusława Łęska, Piotr Przybylski, Bogumil Brzezinski**
Potentiometric and AM1d studies of silicon and boron podands—silver (I) complexes
Journal of Molecular Structure, Volume 788, Issues 1-3, 8 May 2006, Pages 184-189
- **Haggard L**
Selecting desktop molecular modeling software.
Sci Comp & Auto, July 1994.
- **Haiping, Yu, E. Joslin, S.M. Zain, H. Rzepa and D. Phillips**
Normal Modes of 4-aminobenzonitrile (4-ABN). A comparison of PM3 calculations with experimental jet-cooled spectroscopy.
Chemical Physics, Vol. 178, 1993, pp. 483-491.
- **Halton, Brian and Roland Boese and Henry S. Rzepa**
A Molecular Orbital and Crystallographic Study of the Structure and pi-Facial Regioselectivity of 9-Chloro-1,4,5,8-tetrahydro-4a,8a-Methanonaphthalene,
J. Chem. Soc. Perkin Trans. 2, 1992, pp. 447-448.
- **Hanai, Toshihiko, Hatano, Hiroyuki, Nimura, Noriyuki, Kinoshita, Toshia**
Analysis of Chemically Bonded Silica Gel by Computational Chemistry
Journal of Liquid Chromatography, Vol. 16, No. 1., 1993, pp. 109-114
- **Hanai, Toshihiko, Hatano, Hiroyuki, Nimura, Noriyuki, Kinoshita, Toshia**
Chiral Recognition by Chromatography and Computational Chemistry
Journal of Liquid Chromatography, Vol. 16, No. 4, 1993, pp. 801-808.
- **Hanai, Toshihiko, Hatano, Hiroyuki, Nimura, Noriyuki, Kinoshita, Toshia**
Computational Chemical Analysis of the Retention of Saccharides on Amino Phase (Scientific Paper, 1994)
Journal of Liquid Chromatography, Vol. 17, No. 1, 1994, pp. 241-248.
- **Hanai, Toshihiko, Hatano, Hiroyuki, Nimura, Noriyuki, Kinoshita, Toshia**
Enthalpy and Boiling Points in Capillary Column Gas Chromatography
Analytical Sciences, February 1993, Vol. 9, pp. 43-46.

- **Hanai, Toshihiko, Hatano, Hiroyuki, Nimura, Noriyuki, Kinoshita, Toshia,**
QSRR in Liquid Chromatography Aided by Computational Chemistry
Journal of Liquid Chromatography, Vol. 16, No. 7, 1993, pp. 1453-1462.
- **Hanks, T. W., Hallford, R., Wright, G.,**
Examining Host-Guest Interactions with an Integrated Spreadsheet/Molecular-Modeling Program
Journal of Chemical Education, April 1995, Vol. 72, No. 4, pp. 329-332.
- **Hemant Kumar Jain, V.K. Mourya, R.K. Agrawal**
Inhibitory mode of 2-acetoxyphenyl alkyl sulfides against COX-1 and COX-2: QSAR analyses
Bioorganic & Medicinal Chemistry Letters, Volume 16, Issue 20, 15 October 2006, Pages 5280-5284
- **Henderson, Craig C., Cahill, Paul A.**
C₆₀H₂: Synthesis of the Simplest C₆₀ Hydrocarbon Derivative
Science, 26 March 1993, Vol. 259, pp. 1885-1887.
- **Henderson, Craig C., Rohlfing, Celeste McMichael, Gillen, Kenneth T., and Cahill, Paul A.**
C₆₀H₄: Kinetics and Thermodynamics of Multiple Addition to C₆₀
Angewandte Chemie Int. Ed. Engl., Vol. 33, No. 7, 1994, pp. 786-788.
- **Henderson, Craig C., Rohlfing, Celeste McMichael, Gillen, Kenneth T., and Cahill, Paul A.,**
Synthesis, Isolation and Equilibration of 1,9- and 7,8-C₇₀H₂
Science, 15 April 1994, Vol. 264, pp. 397-399.
- **Hickey, Eugene R., Leo A. Paquette**
Experimental and Theoretical Analysis of the Effects of Strain Diminution on the Stereoselectivity of Dienophilic Capture by p-Facially Nonequivalent Homologues of Isodicyclopentadiene
J. Am. Chem. Soc. 1995, 117, 163-176.
- **Hideki Abe, Sakae Aoyagi, and Chihiro Kibayashi,**
First Total Synthesis of the Marine Alkaloids (?)-Fasicularin and (?)-Lepadiformine Based on Stereocontrolled Intramolecular Acylnitroso-Diels-Alder Reaction
Journal of the American Chemical Society; 2000, 122, 4583-4592.
- **Hideyuki Tukada, Katsura Mochizuki**
Crystal structure of 1,3-diphenyladamantane and trans-1,4-diphenylcyclohexane: torsion angles about C-Ph bonds in ?,?-diphenyl(alicyclic hydrocarbon)
Journal of Molecular Structure, Volume 655, Issue 3, 13 August 2003, Pages 473-478
- **Hill, Jameica B., et al.**
Reaction of Me₃Ga and Me₃Al with the Tertiary-Tetraaza Analog of Adamantane, Hexamethylenetetramine (N₄-Ada). Syntheses and Molecular Structures of [(Me₃M)_n N₄-Ada] (n=1-4, M=Ga or Al).
Journal of Organometallic Chemistry, Vol. 445, 1993, pp. 11-18.
- **Hinks, David et al.**
Computer-Aided Dyestuff Design.
Books of Papers for the American Association of Textile Chemists and Colorist Conference and Exhibition on October 7-10, 1995.
- **Hiroaki Gouda, Keiichi Matsuzaki, Haruo Tanaka, and Shuichi Hirono Satoshimura, John A. McCauley, Paul A. Sprengeler, George T. Furst, and Amos B. Smith, III ,**
Stereostructure of (-)-Chloropeptin I, a Novel Inhibitor of gp120-CD4 Binding, via High-Temperature Molecular Dynamics, Monte Carlo Conformational Searching, and NMR Spectroscopy
J. Am. Chem. Soc. 1996, 118(51), 13087-13088.

- **Hiromi Sakurai, Akira Izuoka, and Tadashi Sugawara,**
Design, Preparation, and Electronic Structure of High-Spin Cation Diradicals Derived from Amine-Based Spin-Polarized Donors
Journal of the American Chemical Society; 2000,122, 9723-9734.
- **Hiroshi Imahori, Dirk M. Guldi, Koichi Tamaki, Yutaka Yoshida, Chuping Luo, Yoshiteru Sakata, and Shunichi Fukuzumi**
Charge Separation in a Novel Artificial Photosynthetic Reaction Center Lives 380 ms
Journal of the American Chemical Society; 2001, 123, 6617-6628.
- **Hiroshi Imahori, Kiyoshi Hagiwara, Masanori Aoki, Tsuyoshi Akiyama, Seiji Taniguchi, Tadashi Okada, Masahiro Shirakawa, and Yoshiteru Sakata**
Linkage and Solvent Dependence of Photoinduced Electron Transfer in Zincporphyrin-C60 Dyads
J. Am. Chem. Soc. 1996, 118(47), 11771-11782.
- **Hitoshi Kusama, Mitsuhiko Kurashige, Hironori Arakawa**
Influence of nitrogen-containing heterocyclic additives in I²/I³⁻ redox electrolytic solution on the performance of Ru-dye-sensitized nanocrystalline TiO₂ solar cell
Journal of Photochemistry and Photobiology A: Chemistry, Volume 169, Issue 2, 15 January 2005, Pages 169-176
- **Hofmeister, Gretchen E. and Zhongrui Zhou and Julie A. Leary**
Linkage Position Determination in Lithium-Cationized Disaccharides: Tandem Mass Spectrometry and Semiempirical Calculations.
Journal of the American Chemical Society, Vol. 113, 1991, pp. 5964-5970.
- **Huang, Ming-Ju, Bodor, Nicholas,**
Structural studies of bitetrahedryl molecule C₈H₆, coupled tricyclo [3.1.0.0]hexyl molecule C₁₂H₁₄, and coupled bicyclo[1.1.0]butane derivatives
Chemical Physics Letters, Volume 190, number 1,2, 28 February 1992.
- **Huang, X., D. Marano-Lewicka, R.C. Pfaff, D.E. Nichols,**
Drug Discrimination and Receptor Binding of N-Isopropyl Laysergamide Derivatives.
Pharmacology Biochemistry and Behavior, Vol. 47, No. 3, 1994, pp. 667-673.
- **Huang, Ying, Karen A. Pevear, Mark M. Banaszak Holl, Dwight A. Sweigart, Y.K. Chung**
Ligand Substitution at 19-Electron Organometallic Centers. Electrocatalytic CO substitution reactions of (methylpentadienyl)Mn(CO)₂NO⁺ and (indenyl)Mn(CO)₂NO⁺
Inorganic Chimica Acta., 226, 1994, 53.
- **Huw M. L. Davies, Paul R. Bruzinski, Debra H. Lake, Norman Kong, and Michael J. Fall**
Asymmetric Cyclopropanations by Rhodium(II) N-(Arylsulfonyl)prolinate Catalyzed Decomposition of Vinyl diazomethanes in the Presence of Alkenes. Practical Enantioselective Synthesis of the Four Stereoisomers of 2-Phenylcyclopropan-1-amino Acid
J. Am. Chem. Soc. 1996, 118(29), 6897-6907.
- **Ichihito Narita, Takeo Oku**
Molecular dynamics calculation of H₂ gas storage in C₆₀ and B₃₆N₃₆ clusters
Diamond and Related Materials, Volume 11, Issues 3-6, March-June 2002, Pages 945-948
- **Itoh, Shinobu, Masaki Ogino, Shigenobu Haranou, Tadashi Terasaka, Takeya Ando, Mitsuo Komatsu, Yoshiki Ohshiro, Shunichi Fukuzumi, Kenji Kano, Kazuyoshi Takagi, and Tokuji Ikeda,**
A Model Compound of Novel Cofactor Tryptophan Tryptophylquinone of Bacterial Methylamine Dehydro-genases. Synthesis and Physicochemical Properties
J. Am. Chem. Soc., 1995, 117, 1485-1493.
- **Jadwiga Frelek, Anna Fryszkowska, Marcin Kwit, Ryszard Ostaszewski**
Circular dichroism studies on absolute configuration assignment of peptidomimetics with a

terminal chiral 3-arylpropionic acid unit

Tetrahedron: Asymmetry, Volume 17, Issue 17, 2 October 2006, Pages 2469-2478

- **Jagg, Philip N., et al.**
The Preparation, X-Ray Crystal Structure and Theoretical Study of [CoCp₂][S₃N₃], (Cp=Cyclopentadienyl), a Novel Stacking Compound Incorporating Multiple C-H...N(ppi) Interactions.
J. Chem. Soc., Chemical Communications, Issue 14, 1991.
- **Jaromir Kira, Bogusława Łęska, Grzegorz Schroeder, Piotr Przybylski, Bogumił Brzezinski**
Potentiometric and AM1d studies of silicon podands—silver(I) complexes
Journal of Molecular Structure, Volume 738, Issues 1-3, 14 March 2005, Pages 227-231
- **Jaromir Kira, Bogusława Łęska, Oksana Nevecheriya, Grzegorz Schroeder, Piotr Przybylski, Bogumil Brzezinski**
Potentiometric and AM1d studies of silicon and phosphorous podands-silver (I) complexes
Journal of Molecular Structure, Volume 749, Issues 1-3, 15 July 2005, Pages 122-127
- **Jayna Chan, Zuyun Huang, Maureen E. Merrifield, Maria T. Salgado, Martin J. Stillman**
Studies of metal binding reactions in metallothioneins by spectroscopic, molecular biology, and molecular modeling techniques
Coordination Chemistry Reviews, Volumes 233-234, 1 November 2002, Pages 319-339
- **Jeffrey K. Politis, Joel C. Nemes, and M. David Curtis**
Synthesis and Characterization of Regiorandom and Regioregular Poly(3-octylfuran)
Journal of the American Chemical Society; 2001,123, 2537-2547.
- **Jeliazko G. Polihronov, Magnus Hedstr om, Rolf E. Hummel, Hai-Ping Cheng**
Semi-empirical calculation of the optical spectra of silica clusters in spark-processed silicon
Journal of Luminescence, Volume 96, Issues 2-4, March 2002, Pages 119-128
- **Jeong, Jae Uk and P.L. Fuchs,**
Spiroketal Equilibration: Interconversion of 1,6-Dioxaspiro[4.4]nonanes and 1,6-Dioxaspiro[4.5]decanes. Implications for the Synthesis of Cephalostatin 7.
Tetrahedron Letters, Vol. 35, No. 30, 1995, pp. 5385-5388.
- **Jeong, Jae Uk and P.L. Fuchs,**
Synthesis of the South Hexacyclic Steroid Unit of Cephalostatin 7.
Tetrahedron Letters, Vol. 36, No. 14, 1995, pp. 2431-2434.
- **Jin Mizuguchi, Kazuyuki Hino, Kaoru Tojo**
Strikingly different electronic spectra of structurally similar perylene imide compounds
Dyes and Pigments, Volume 70, Issue 2, 2006, Pages 126-135
- **Joanna Kurek, Władysław Boczon, Piotr Przybylski, Bogumił Brzezinski**
ESI MS, spectroscopic and PM5 semiempirical studies of Colchicine complexes with lithium, sodium and potassium salts
Journal of Molecular Structure, Volume 846, Issues 1-3, 26 November 2007, Pages 13-22
- **John Mack, Martin J. Stillman, Nagao Kobayashi**
Application of MCD spectroscopy to porphyrinoids
Coordination Chemistry Reviews, Volume 251, Issues 3-4, February 2007, Pages 429-453
- **John Watts, Alex Benn, Nick Flinn, Tracy Monk, Manoj Ramjee, Peter Ray, Yikang Wang, Martin Quibell**
Functionalised 2,3-dimethyl-3-aminotetrahydrofuran-4-one and N-(3-oxo-hexahydrocyclopenta[b]furan-3a-yl)acylamide based scaffolds: synthesis and cysteinyl proteinase inhibition
Bioorganic & Medicinal Chemistry, Volume 12, Issue 11, 1 June 2004, Pages 2903-2925

- **Johnston, Andrew G., David A. Leigh, Robin J. Pritchard and Michael D. Deegan,**
Facile Synthesis and Solid-State Structure of a Benzylic Amide [2]Catanane.
Angewandte Chemie International Ed. English, Vol. 34, No. 11, 1995, S.1209-1216.
- **Joseph W. Toporowski, Swarnalatha Y. Reddy, Thomas C. Bruice**
An investigation of the ionic and solvation patterns of dsDNG versus dsDNA by use of molecular dynamics simulations
Biophysical Chemistry, Volume 126, Issues 1-3, March 2007, Pages 132-139
- **Julio A. Seijas, M. Pilar Vázquez-Tato, M. Montserrat Martínez, Moacir G. Pizzolatti**
Oxazoline as a useful tool in organic synthesis: preparation of 4-aryl-1,2,3,4-tetrahydroisoquinoline alkaloid skeleton
Tetrahedron Letters, Volume 46, Issue 35, 29 August 2005, Pages 5827-5830
- **Katja Miettinen, Elina Vuorimaa, Stefano Cattaneo, Alexandre Efimov, Helge Lemmetyinen, Martti Kauranen**
Effect of the deposition type on the structure of terthiophene-vinylbenzoate Langmuir–Blodgett films
Thin Solid Films, In Press, Corrected Proof, Available online 4 April 2008
- **Kazunori Tsubaki, Dinh T.T. Hai, Valluru K. Reddy, Hiroshi Ohnishi, Kaoru Fuji, Takeo Kawabata**
Synthesis of chiral 2,2'-dimethyl-1,1'-binaphthyl-8,8'-diamine and barriers of atropisomerization of the related binaphthyls
Tetrahedron: Asymmetry, Volume 18, Issue 8, 16 May 2007, Pages 1017-1021
- **Kei Maekawa, Norikazu Hishikawa, Kanji Kubo, Tetsutaro Igarashi, Tadimitsu Sakurai**
Preferential formation of cis-4,5-dihydrooxazole derivatives via photoinduced electron transfer-initiated cyclization of N-acyl- α -dehydroaryllalanine alkyl esters
Tetrahedron, Volume 63, Issue 46, 12 November 2007, Pages 11267-11281
- **Keiichi Kimura, Ryoko Mizutani, Masaaki Yokoyama, Ryuichi Arakawa, and Yoshiaki Sakurai,**
Metal-Ion Complexation and Photochromism of Triphenylmethane Dye Derivatives Incorporating Monoaza-15-crown-5 Moieties
Journal of the American Chemical Society; 2000; 122, 5448-5454.
- **Kentaro Miyoshi, Kazuya Uezu, Kazuo Sakurai, Seiji Shinkai**
Inter-chain and arrayed hydrogen bonds in α -1,3-d-xylan triple helix predicted by quantum mechanics calculation
Carbohydrate Polymers, Volume 66, Issue 3, 2 November 2006, Pages 352-356
- **Kenzi Hori, Kazuaki Yoshimura, Hidetoshi Ohno, Kenjiro Onimura, Tsutomu Oishi**
Theoretical study on the polymerization mechanism of substituted maleimides by using a chiral catalyst with Zn²⁺
Tetrahedron, Volume 59, Issue 33, 11 August 2003, Pages 6301-6309
- **Kinoshita, Toshia, Miyayama, Miyoko, Kyodo, Yukiko, Kamitani, Yochie, Miyamasu, Misato, Nimura, Noriyuki, Hanai, Toshihiko**
Study of Chemobiological Reactions. 1. Selectivity of Aromatic Amino Compounds and Saccharids in Glycosylation Reactions
Biomedical Chromatography, Vol. 7, 1993, 64-67.
- **Kogan, Timothy P., B. Mitch Revelle, S. Tapp, D. Scott, P.J. Beck,**
A Single Amino Acid Residue Can Determine the Ligand Specificity of E-selectin.
The Journal of Biological Chemistry, Vol. 270, No. 23, 1995, pp. 14047-14055.
- **Krishna Kumar, Zhe Lin, David H. Waldeck, and Matthew B. Zimmt**
Electronic Coupling in C-Clamp-Shaped Molecules: Solvent-Mediated Superexchange

Pathways

J. Am. Chem. Soc. 1996, 118(1), 243-244.

- **Kurosawa, Shigeru, Sekiya, Akira, Shibakami, Motonari, Tamura, Masanori, Arimura, Takashi**
Semi-empirical Molecular Orbital Studies of Monofluorination reactions: Reaction of Hydrofluorocarbons Over Cobalt Trifluoride
Journal of Fluorine Chemistry, 70, 1995, pp. 49-52.
- **Laurent Djakovitch and Klaus Koehler**
Heck Reaction Catalyzed by Pd-Modified Zeolites
Journal of the American Chemical Society; 2001, 123, 5990-5999.
- **Le, Thao D. and Jeffrey G. Weers,**
QSPR and GCA Models for Predicting the Normal Boiling Points of Fluorocarbons.
The Journal of Physical Chemistry, Vol. 99, No. 17, 1995, pp. 6739-6747.
- **Leary, Julie A., et al.**
Investigations of Gas-Phase Lithium-Peptide Adducts: Tandem Mass Spectrometry and Semiempirical Studies.
Journal American Society for Mass Spectrometry, 1990, pp. 473-480.
- **Lee, Moses, Garbiras, Bonnie, and Preti, Christopher**
An Undergraduate Organic Synthesis, Spectroscopy, and Molecular Modeling Project
Journal of Chemical Education, April 1995, Vol. 72, No. 4, pp. 378-380.
- **Lee, Sunghee, Sanjeev Makan, Mark M. Banaszak Holl, F. Read McFeely,**
Synthetic Control of Solid/Solid Interfaces: Analysis of Three New Silicon/Silicon Oxide Interfaces by Soft X-Ray Photoemission.
J. Am. Chem. Soc., Vol. 116, 1994, 11819.
- **Lewis, Nita A., Friesen, Christian, White, Peter S.**
Use of Extended Hueckel Molecular Orbital Calculations in Determining the Position of Attack in Inner-Sphere Electron-Transfer Reactions: X-ray Crystal Structure of (1,3-Diphenylpropane-1,3-dionato)bis(ethylenediamine)cobalt(III)
Inorganic Chemistry, Vol. 27, 1988, 1662.
- **Li, Wen, Carl C. Wamser**
Synthesis and Characterization of Interfacially Polymerized Films of Tetraphenylporphyrin Derivatives.
Published by Department of Chemistry, Portland State University.
- **Li-Rung Chen, Yu-Chin Wang, Yi Wen Lin, Shan-Yen Chou, Shyh-Fong Chen, Lee Tai Liu, Ying-Ta Wu, Chih-Jung Kuo, Tom Shieh-Shung Chen, Shin-Hun Juang**
Synthesis and evaluation of isatin derivatives as effective SARS coronavirus 3CL protease inhibitors
Bioorganic & Medicinal Chemistry Letters, Volume 15, Issue 12, 15 June 2005, Pages 3058-3062
- **Li-Xian Sun, Naoki Matsuda, Akiko Takatsu, Kenji Kato, Tatsuhiko Okada**
Study of adsorption of methylene blue and new methylene blue in liquid–solid interface by slab optical waveguide spectroscopy
Talanta, Volume 65, Issue 5, 15 March 2005, Pages 1143-1148
- **Li-Xian Sun, Tatsuhiko Okada**
Studies on interactions between Nafion and organic vapours by quartz crystal microbalance
Journal of Membrane Science, Volume 183, Issue 2, 1 March 2001, Pages 213-221
- **Louraine C. de Melo, Scheila F. Braga, P.M.V.B. Barone**
Pattern recognition methods investigation of ellipticines structure–activity relationships

Journal of Molecular Graphics and Modelling, Volume 25, Issue 6, March 2007, Pages 912-920

- **M. Kwit, J. Gawronski**
Chiral calixsalen-type macrocycles from trans-1,2-diaminocyclohexane
Tetrahedron: Asymmetry, Volume 14, Issue 10, 16 May 2003, Pages 1303-1308
- **M. Kwit, J. Gawronski**
Helicity of N,N'-diaryl-trans-1,2-diaminocyclohexane derivatives. Implications for molecular helicity manipulations
Tetrahedron, Volume 59, Issue 47, 17 November 2003, Pages 9323-9331
- **M. Walkowiak, G. Schroeder, B. Gierczyk, D. Waszak, M. Osinska**
New lithium ion conducting polymer electrolytes based on polysiloxane grafted with Si-tripodand centers
Electrochemistry Communications, Volume 9, Issue 7, July 2007, Pages 1558-1562
- **Magdalena Capó**
31P NMR spectroscopy and discrete metallocycles from non-rigid ligands
Polyhedron, Volume 27, Issue 5, 7 April 2008, Pages 1329-1332
- **Magdalena Miernicka, Agata Szulawska, Malgorzata Czyz, Ingo-Peter Lorenz, Peter Mayer, Boleslaw Karwowski, Elzbieta Budzisz**
Cytotoxic effect, differentiation, inhibition of growth and theoretical calculations of an N,N-donor ligands and its platinum(II), palladium(II) and copper(II) complexes
Journal of Inorganic Biochemistry, Volume 102, Issue 2, February 2008, Pages 157-165
- **Makoto Fujita, Fumiaki Ibukuro, Hiroko Seki, Osamu Kamo, Mamoru Imanari, and Katsuyuki Ogura,**
Catenane Formation from Two Molecular Rings through Very Rapid Slippage. A Mobius Strip Mechanism.
J. Am. Chem. Soc. 1996, 118(4), 899-900.
- **Malwitz, Nelson**
Polyurethane Reactions According to Computational Chemistry
Cellular Polymers III, 1995.
- **Malwitz, Nelson**
Reaction Kinetic Modeling from PM3 Transition State Calculations
The Journal of Physical Chemistry, 1995, 99.
- **Malwitz, Nelson,**
Polyurethane Formulation by Computational Chemistry.
Published by Rappa Technology Ltd., Book of Papers from a two-day conference, 27-28 April, 1995.
- **Malwitz, Nelson, Frisch, K.C., Eldred, E.W.,**
Polyurethane Formulation by Computational Chemistry.
25th Anniversary Symposium of the Polymer Institute, September, 1994.
- **Manabendra Ray, Adina P. Golombek, Michael P. Hendrich, Victor G. Young, Jr., and A. S. Borovik**
Synthesis and Structure of a Trigonal Monopyramidal Fe(II) Complex and Its Paramagnetic Carbon Monoxide Derivative
J. Am. Chem. Soc. 1996, 118(25), 6084-6085.
- **Manabu Abe, Kiyotada Fujimoto, and Masatomo Nojima,**
Notable Sulfur Atom Effects on the Regio- and Stereoselective Formation of Oxetanes in Patern?-Böchi Photocycloaddition of Aromatic Aldehydes with Silyl O,S-Ketene Acetals
Journal of the American Chemical Society; 2000,122, 4005-4010.

- **Márcia Valéria Gaspar de Araújo, Elze Kelly Barbosa Vieira, Gilderman Silva Lázaro, Leila de Souza Conegero, Odair Pastor Ferreira, Luí's Eduardo Almeida, Ledjane Silva Barreto, Nivan Bezerra da Costa Jr., Iara F. Gimenez**
 Inclusion complexes of primethamine in 2-hydroxypropyl- β -cyclodextrin: Characterization, phase solubility and molecular modelling
Bioorganic & Medicinal Chemistry, Volume 15, Issue 17, 1 September 2007, Pages 5752-5759
- **Márcia Valéria Gaspar de Araújo, Elze Kelly Barbosa Vieira, Gilderman Silva Lázaro, Leila Souza Conegero, Luís Eduardo Almeida, Ledjane Silva Barreto, Nivan Bezerra da Costa Jr., Iara F. Gimenez**
 Sulfadiazine/hydroxypropyl- β -cyclodextrin host-guest system: Characterization, phase-solubility and molecular modeling
Bioorganic & Medicinal Chemistry, Volume 16, Issue 10, 15 May 2008, Pages 5788-5794
- **Marcin Kwit, Jacek Gawronski**
 A circular dichroism detection of stereostructural change due to amine protonation
Tetrahedron Letters, Volume 44, Issue 45, 3 November 2003, Pages 8311-8314
- **Marko Strukelj, Rebecca H. Jordan, and Ananth Dodabalapur**
 Organic Multilayer White Light Emitting Diodes
J. Am. Chem. Soc. 1996, 118(5), 1213-1214.
- **Marshall G. Cory and Michael C. Zerner ,**
 Calculation of the Electron Affinities of the Chromophores Involved in Photosynthesis
J. Am. Chem. Soc. 1996, 118(17), 4148-4151.
- **Martin Quibell, Alex Benn, Nick Flinn, Tracy Monk, Manoj Ramjee, Yikang Wang, John Watts**
 Bicyclic peptidomimetic tetrahydrofuro[3,2-b]pyrrol-3-one and hexahydrofuro[3,2-b]pyridine-3-one based scaffolds: synthesis and cysteinyl proteinase inhibition
Bioorganic & Medicinal Chemistry, Volume 12, Issue 21, 1 November 2004, Pages 5689-5710
- **Maruoka, Keiji, Susumu Saito and Hisashi Yamamoto,**
 Molecular Design of a Chiral Lewis Acid for the Asymmetric Claisen Rearrangement
J. Am. Chem. Soc. 1995, 117(3), 1165-1166.
- **Masaru Yoshida, Midori Goto, Fusae Nakanishi**
 Synthesis, structures, and conformational analysis of dibenzodioxadisilocins
Inorganic Chemistry Communications, Volume 3, Issue 2, 1 February 2000, Pages 59-61
- **Mateo Alajarin, Carlota Conesa and Henry S. Rzepa,**
 Ab initio SCF-MO study of the Staudinger phosphorylation reaction between a phosphane and an azide to form a phosphazene
J. Chem. Soc., Perkin Trans. 2, 1999, 1811-1814. Received (in Cambridge, UK) 4th June 1999, Accepted 7th July 1999.
- **McClain, Mark D., M.S. Hay, M.D. Curtis, J.W. Kampf,**
 Structure, Reactivity, and an EHMO Analysis of a Metal-Stabilized Dicarbenium Ion, [Cp₂Mo₂(CO)₄(CH₂CCCH₂)](BF₄)₂.
Organometallics, Vol 13, No. 11, 1994, pp. 4377-4386.
- **Mebane, Robert C., Mary J. Gray, et al.,**
 Molecular Modelings and Molecular Cross-Sectional Areas: A Comparison with Molecules Adsorbed on Solid Surfaces.
J. of Colloid and Interface Science, Vol. 170, 1995, pp. 98-101.
- **Megumi Kobayashi, Sentaro Okamoto**
 Unexpected reactivity of annulated 3H-benzothiazol-2-ylideneamines as an acyl transfer catalyst
Tetrahedron Letters, Volume 47, Issue 26, 26 June 2006, Pages 4347-4350

- **Melina Monasterios, Marilu Escorche, Milagros Avenda?o**
Conformational analysis, electronic properties and molecular electrostatic potential of nitrofurans derivatives with antibacterial activity
Journal of Molecular Structure, Volume 748, Issues 1-3, 30 June 2005, Pages 49-55
- **Melina Monasterios, Milagros Avenda?o, María Isabel Amaro, Wilson Infante, Jaime Charris**
Relation between molecular electrostatic potential, several electronic properties and antibacterial activity of some synthetic furane derivatives
Journal of Molecular Structure, Volume 798, Issues 1-3, 23 October 2006, Pages 102-108
- **Minati Baral, Suban K. Sahoo, B.K. Kanungo**
Tripodal amine catechol ligands: A fascinating class of chelators for aluminium(III)
Journal of Inorganic Biochemistry, In Press, Corrected Proof, Available online 4 March 2008
- **Moloy, Kenneth G. and Jeffrey L. Petersen,**
N -Pyrrolyl Phosphines: An Unexploited Class of Phosphine Ligands with Exceptional p-Acceptor Character
J. Am. Chem. Soc. 1995, 117, 7696-7710.
- **Murray, Henry H., Liwen Wei, Suzanne Sherman, Mark Greaney, Kenneth Ericksen, Barbara Carstensen, Thomas Halbert, Edward Steifel,**
Induced Internal Electron Transfer Chemistry in Rhenium Sulfide Systems.
Inorganic Chemistry, Vol. 34, 1995, pp. 841-853.
- **Mutsumi Ohkubo, Wataru Uchikawa, Hitomi Matsushita, Aiko Nakano, Takayuki Shirato, Sentaro Okamoto**
Stereoselective construction of 3a-methylhydrindanes starting from 2,7-enynol derivatives based on Ti(II)-mediated cyclization and Ru-catalyzed ring-closing metathesis
Tetrahedron Letters, Volume 47, Issue 29, 17 July 2006, Pages 5181-5185
- **Nataliya Lyapchenko, Grzegorz Schroeder, Piotr Przybylski, Agnieszka Burzynska, Paweł Kafarski, Bogumił Brzezinski**
Mass spectrometric and PM5 study of some piperidine-N-methyldiphosphonic acids and their complexes with alkali cations
Journal of Molecular Structure, Volume 782, Issues 2-3, 23 January 2006, Pages 183-190
- **Nikolay Gerasimchuk, Leon Goeden, Paul Durham, Charles Barnes, John F. Cannon, Svitlana Silchenko, Ismael Hidalgo**
Synthesis and characterization of disubstituted arylcyanoximes and their several metal complexes
Inorganica Chimica Acta, Volume 361, Issue 7, 20 May 2008, Pages 1983-2001
- **Novick, S.G., Godfrey, J.C., Godfrey, N.J., Wilder, H.R.**
How Does Zinc Modify the Common Cold?
Medical Hypotheses, (1996) Vol. 46, pp. 295-302.
- **Novoa, Juan J. and Myung-Hwan Whangbo**
The Nature of Intramolecular Hydrogen-Bonded and Non-Hydrogen-Bonded Conformations of Simple Di- and Triamides.
Journal of the American Chemical Society, Vol. 113, No. 24, November 20, 1991.
- **Oberlender, Robert, et al.**
Stereoselective LSD-like Activity in d-Lysergic Acid Amides of (R)- and (S)-2-Aminobutane.
Journal of Medicinal Chemistry, Vol. 35, No. 2, January 24, 1992, pp. 203-211.
- **Ogawa-K Nakata-K Ichikawa-K**
Molecular-Structures of Zinc-Complexes with Bisbenzimidazole Ligands in Crystals and the Kinetics of Ligand-Exchange Reactions in Their Solutions
Bulletin of the Chemical Society of Japan 1997, 70, p 2925-2933.

- **Ohta, Kazuo, Miyagawa, Osamu, Tsutsui, Hironori, Mitsunobu, Oyo,**
Total Synthesis of Grahamimycin A1.
Bull. Chem. Soc. Jpn., Vol. 66, 1993, pp. 523-535.
- **Padwa, Albert, D. Austin, A. Price, M. Semones, M. Doyle, M. Protopopova, W. Wichester, A. Tran**
Ligand Effects on Dirhodium(II) Carbene Reactivities. Highly Effective Switching between Competitive Carbenoid Transformations.
Journal of the American Chemical Society, Vol. 115. Mp; 19. 1993, pp. 8669-8680.
- **Peter Leeming, Colin A. Ray, Stephen J. Simpson, Timothy W. Wallace, Richard A. Ward**
Stereoselective routes to substituted β -amino carbonyl compounds via heterodiene [4+2?] cycloadditions of auxiliary-based C2 symmetric ketene acetals
Tetrahedron, Volume 59, Issue 3, 13 January 2003, Pages 341-352
- **Pevear, Karen A., Mark M. Banaszak Holl, Gene B. Carpenter, Anne L. Rieger, Phillip H. Rieger, Dwight A. Sweigart**
Ligand Substitution at 19-Electron Centers and the Idenyl Effect in Organometallic Radicals. Electrocatalytic CO substitution in (Cyclopentadienyl)Fe(CO)₃⁺ and (Indenyl)Fe(CO)₃⁺
Organometallics, Vol. 14, 1995, pp. 512-523.
- **Piotr Przybylski, Adam Huczynski, Bogumil Brzezinski**
The structures of monensin A derivatives and its complexes with some monovalent cations studied by the AM1d, PM3 as well as PM5 semiempirical methods
Journal of Molecular Structure, Volume 826, Issues 2-3, 29 January 2007, Pages 156-164
- **Piotr Przybylski, Adam Huczynski, Małgorzata Wichłacz, Małgorzata Ratajczak-Sitarz, Andrzej Katrusiak, Bogumil Brzezinski**
Spectroscopic, semiempirical and X-ray structural study of the 2:1 complex of a cyclic diamide of o-phthalic acid with water molecule
Journal of Molecular Structure, Volume 840, Issues 1-3, 17 September 2007, Pages 22-28
- **Piotr Przybylski, Beata Kołodziej, Grzegorz Leniec, Sławomir M. Kaczmarek, Eugeniusz Grech, Janusz Typek, Bogumil Brzezinski**
ESI MS, spectroscopic and semiempirical characterization of a macrobicyclic complex with Er (III) cation
Journal of Molecular Structure, Volume 878, Issues 1-3, 30 April 2008, Pages 95-103
- **Piotr Przybylski, Bogumil Brzezinski, Franz Bartl**
Oligomycin A complex structures with some divalent metal cations studied by ESI MS and PM5 semiempirical methods
Journal of Molecular Structure, Volume 830, Issues 1-3, 30 March 2007, Pages 58-71
- **Piotr Przybylski, Bogumił Brzezinski, Franz Bartl**
Spectroscopic and PM5 studies of a new Schiff base of Gossypol with 4?-aminobenzo-15-crown-5 in solution
Journal of Molecular Structure, Volume 794, Issues 1-3, 7 August 2006, Pages 237-243
- **Piotr Przybylski, Grzegorz Bejcar, Wojciech Schilf, Bogumil Brzezinski**
Structural and semiempirical investigation of hydrazone of gossypol and its protonated species
Journal of Molecular Structure, Volume 878, Issues 1-3, 30 April 2008, Pages 71-77
- **Piotr Przybylski, Grzegorz Schroeder, Bogumil Brzezinski**
The Schiff base of gossypol with 2-(aminomethyl)-18-crown-6 complexes and H⁺, Li⁺, Na⁺, K⁺, Rb⁺, Cs⁺ cations studied by ESI MS, 1H NMR, FT-IR and PM5 semiempirical methods
Journal of Molecular Structure, Volume 699, Issues 1-3, 2 August 2004, Pages 65-77
- **Piotr Przybylski, Krystian Pyta, Barbara Wicher, Maria Gdaniec, Bogumił Brzezinski**
Structure of a new Schiff base of gossypol with 1-(3-aminopropyl)-2-pyrrolidinone studied by

the X-ray, FT-IR, NMR, ESI-MS and PM5 methods

Journal of Molecular Structure, In Press, Corrected Proof, Available online 29 February 2008

- **Piotr Przybylski, Magdalena Wodarz, Bogumil Brzezinski, Franz Bartl**
Spectroscopic studies and PM5 semiempirical calculations of tautomeric forms of gossypol schiff base with (R)-tetrahydrofurfurylamine
Journal of Molecular Structure, Volume 691, Issues 1-3, 29 March 2004, Pages 227-234
- **Piotr Przybylski, Magdalena Wodarz, Grzegorz Schroeder, Radosaw Pankiewicz, Bogumil Brzezinski, Franz Bartl**
ESI MS and PM5 semiempirical studies of gossypol schiff base with (R)-tetrahydrofurfurylamine complexes and monovalent cations
Journal of Molecular Structure, Volume 693, Issues 1-3, May 2004, Pages 95-102
- **Piotr Przybylski, Maria Małuszynska, Bogumił Brzezinski**
Spectroscopic and semiempirical studies of new Schiff base of gossypol with allylamine in solution
Journal of Molecular Structure, Volume 750, Issues 1-3, 15 August 2005, Pages 152-157
- **Piotr Przybylski, Weronika Lewandowska, Bogumił Brzezinski, Franz Bartl**
1H, 13C and 15N NMR, FT-IR as well as PM5 studies of a new Schiff base of gossypol with 3,6-dioxadecylamine in solution
Journal of Molecular Structure, Volume 797, Issues 1-3, 18 September 2006, Pages 92-98
- **Piotr Przybylski, Wojciech Schilf, Bogumił Brzezinski**
13C, 15N NMR and CP-MAS as well as FT-IR and PM5 studies of Schiff base of gossypol with l-phenylalanine methyl ester in solution and solid
Journal of Molecular Structure, Volume 734, Issues 1-3, 31 January 2005, Pages 123-128
- **Piotr Przybylski, Wojciech Schilf, Bohdan Kamienski, Bogumil Brzezinski, Franz Bartl**
13C, 15N CP-MAS, FT-IR and PM5 studies of some Schiff bases of gossypol in solid
Journal of Molecular Structure, Volume 748, Issues 1-3, 30 June 2005, Pages 111-117
- **Pop, Emil, Brewster, Marcus, E., Dinculescu, Antoinie, Huang, Ming-Ju, Bodor, Nicholas**
Isomerism of Cephalosporin esters; Theoretical and Practical Aspects
Heterocycles, Vol. 37, No. 1, 1994.
- **Pop, Emil, Brewster, Marcus, E., Huang, Ming-Ju, Bodor, Nicholas**
Dihydropyridine Isomerism in the Chemical Delivery System Series
CROATICA CHEMICA ACTA, CCACAA 66 (3-4) 531-537 (1993).
- **Pop, Emil, Brewster, Marcus, E., Huang, Ming-Ju, Bodor, Nicholas**
Dithionite reduction of pyridinium salts: an AM1 study
Journal of Molecular Structure (Theochem), 283 (1993) 27-32.
- **Pop, Emil, et al.**
A Theoretical Study of the Hydrolysis of Some Sterically Hindered Phenolic Esters.
International Journal of Quantum Chemistry: Quantum Biology Symposium 19, 1992, pp. 77-85.
- **Pop, Emil, et al.**
Electrophilic Substitution in the Benzofuran Series: A Theoretical (AM1) Study.
International Journal of Quantum Chemistry: Quantum Chemistry Symposium 25, 1991, pp. 325-333.
- **Pop, Emil, Huang, Ming-Ju, Bodor, Nicholas, Bercovici, Sorin and Shatzmiller, Shimon**
Ionic and radical intermediates of 3-substituted 5,6-dihydro-1,4,2-dioxazines: a theoretical (AM1) study.
Journal of Molecular Structure (Theochem), 235, (1991) 343-353.

- **Purvis III, George D.**
On the Use of Isovalued Surfaces to Determine Molecule Shape and Reaction Pathways.
Journal of Computer-Aided Molecular Design, Vol. 5, 1991, pp. 55-80.
- **Purvis, George D. III**
The Chemical Sample: A Fundamental Object for Molecular Modeling
Journal of Chemical Information and Computer Sciences, 1994, 34.
- **R. Vendrame, V.R. Coluci, D.S. Galvão**
Comparative parametric method 5 (PM5) study of trans-stilbene
Journal of Molecular Structure: THEOCHEM, Volume 686, Issues 1-3, 25 October 2004, Pages 103-108
- **Radosaw Pankiewicz, Aleksandra Pawowska, Grzegorz Schroeder, Piotr Przybylski, Bogumi Brzezinski, Franz Bartl**
Multinuclear NMR, FT-IR, ESI MS studies and PM5 semiempirical calculations of new ethylene glycol ester of lasalocid acid and their complexes with K⁺ cation
Journal of Molecular Structure, Volume 694, Issues 1-3, June 2004, Pages 55-61
- **Radosaw Pankiewicz, Aleksandra Pawowska, Grzegorz Schroeder, Piotr Przybylski, Bogumi Brzezinski, Franz Bartl**
NMR, FT-IR, ESI MS studies and PM5 semiempirical calculations of lasalocid ethylene glycol ester complexes with Li⁺ and Na⁺ cations
Journal of Molecular Structure, Volume 694, Issues 1-3, June 2004, Pages 155-163
- **Radosław Pankiewicz, Dorota Remlein-Starosta, Grzegorz Schroeder, Bogumił Brzezinski**
Biological activity and ESI MS study of oxaalkyl and hydroksyoxaalkyl lasalocid esters
Journal of Molecular Structure, Volume 783, Issues 1-3, 6 February 2006, Pages 136-144
- **Radosław Pankiewicz, Grzegorz Schroeder, Bogumił Brzezinski**
Spectroscopic and PM5 semiempirical study of a new lasalocid ester with 2-allyloxyethanol and its complexes with monovalent cations
Journal of Molecular Structure, Volume 789, Issues 1-3, 22 May 2006, Pages 1-7
- **Radosław Pankiewicz, Grzegorz Schroeder, Bogumił Brzezinski**
NMR, FT-IR, ESI MS and PM5 semiempirical study of new lasalocid 5-hydroxy-3-oxapentyl ester and its complexes with monovalent cations
Journal of Molecular Structure, Volume 733, Issues 1-3, 3 January 2005, Pages 155-165
- **Radosław Pankiewicz, Grzegorz Schroeder, Bogumił Brzezinski**
Spectroscopic, spectrometric and PM5 semiempirical investigation of new lasalocid 8-hydroxy-3,6-dioxaoctyl ester and its complexes with monovalent cations
Journal of Molecular Structure, Volume 733, Issues 1-3, 3 January 2005, Pages 217-229
- **Radoslaw Pankiewicz, Grzegorz Schroeder, Bogumil Brzezinski, Franz Bartl**
Spectroscopic and PM5 semiempirical study of new lasalocid 5-hydroxypentyl ester and its complexes with monovalent cations
Journal of Molecular Structure, Volume 699, Issues 1-3, 2 August 2004, Pages 53-64
- **Radosław Pankiewicz, Jaromir Kira, Grzegorz Schroeder, Tadeusz Ossowski, Bogumił Brzezinski**
Potentiometric, ESI MS and AM1d studies of lasalocid esters–silver(I) complexes
Journal of Molecular Structure, Volume 782, Issues 2-3, 23 January 2006, Pages 73-80
- **Ramadan A. Bawa, Simon Jones**
Synthesis and Diels–Alder reactions of 9-(4-benzyloxazolin-2-yl) anthracene
Tetrahedron, Volume 60, Issue 12, 15 March 2004, Pages 2765-2770
- **Reilly, Sean D., Carl C. Wamser**
Reactions of Methylene with Hexamethyl (Dewar benzene).
J. Organic Chemistry, Vol. 56, No. 17, 1991, pp. 5232-5234.

- **Ren?e Shediac, Mike H. B. Gray, H. Tetsuo Uyeda, Robert C. Johnson, Joseph T. Hupp, Paul J. Angiolillo, and Michael J. Therien,**
Singlet and Triplet Excited States of Emissive, Conjugated Bis(porphyrin) Compounds Probed by Optical and EPR Spectroscopic Methods
Journal of the American Chemical Society; 2000,122, 7017-7033.
- **Riyako Ikeda, Yuji Soneta, Kazuo Miyamura**
First X-ray structure of a trans-IV of Ni complex of tetra-azamacrocycles with pendent groups, 1,8-bis(N,N-dimethylcarbamoylethyl)-1,5,8,12-tetramethyl-1,4,8,11-tetraazacyclotetra-decane
Inorganic Chemistry Communications, Volume 10, Issue 5, May 2007, Pages 590-592
- **Ronald L. Musselman**
Solid-state spectral perturbations in square-planar complexes
Inorganica Chimica Acta, Volume 361, Issue 4, 3 March 2008, Pages 820-830
- **Rupinder K. Lota, Sachin Dhanani, Caroline P. Owen, Sabbir Ahmed**
Synthesis, biochemical evaluation and rationalisation of the inhibitory activity of a series of 4-hydroxyphenyl ketones as potential inhibitors of 17?-hydroxysteroid dehydrogenase type 3 (17?-HSD3)
Bioorganic & Medicinal Chemistry Letters, Volume 16, Issue 17, 1 September 2006, Pages 4519-4522
- **Ruth W. Kaplan, Andrew M. Napper, David H. Waldeck, and Matthew B. Zimmt**
Solvent Mediated Coupling Across 1 nm: Not a Bond in Sight
Journal of the American Chemical Society; 2000,122, 12039-12040.
- **Rybolt, Thomas R. and C.L. McConnell,**
Calculations of Henry's Law Constants for Adsorption of Aromatic Hydrocarbons on a Graphitic Carbon Surface.
J. of Tennessee Academy of Science, Vol. 69, No. 1, 1994, pp. 1-6.
- **Rzepa, Henry S. and G.A. Suner**
Theoretical Calculations of Benzoquinone Redox Potentials using the COSMO Continuum Solvation Model.
J. Chem. Soc., Chemical Communications, Issue 23, 1993, pp.1743-1774.
- **Rzepa, Henry S. and Man Yin Yi**
An AM1 and PM3 Molecular Orbital and Self-Consistent Reaction-Field Study of the Aqueous Solvation of Glycine, Alanine and Proline in their Neutral and Zwitterionic Forms.
J. Chem. Soc., Perkin Trans., Issue 2, 1991, pp. 531-537.
- **Rzepa, Henry S. and William A. Wylie**
Transition State Structure in Cycloaddition Reactions as a Function of Ring Size and Geometry.
J. Chem. Soc., Perkin Trans., Issue 2, 1991, pp. 939-946.
- **Rzepa, Henry S. et al.**
A Crystallographic, AM1 and PM3 SCF-MO Investigation of strong OH n-Alkene and Alkyne Hydrogen Bonding Interactions.
J. Chem. Soc., Perkin Transaction 2, 1994, pp. 703-707.
- **Rzepa, Henry S. et al.**
A Molecular Orbital and S-Crystallographic Study of the Structure and n-Facial Regioselectivity of 9-Chloro-1,4,5,8-tetrahydro-4a, 8a-methanonaphthalene.
J. Chem. Soc., Perkin Transaction 2, Issue 4, 1992, pp. 447-448.
- **Rzepa, Henry S. et al.**
An AM1 and PM3 Molecular Orbital Study of the Pericyclic Reactivity of Aryl Carbodiimides.
Tetrahedron, Vol. 48, 1992, No. 36, pp. 7425-7434.

- **Rzepa, Henry S. et al.**
An MCSF Study of the Effect of Substituents and Solvent on the [2+2]Cycloaddition of tert-Butyrcyanoketene to Phenylethene.
J. Chem. Soc., Perkin Transaction 2, 1993, pp. 1499-1502.
- **Rzepa, Henry S. et al.**
An Unusual Example of Stereoelectronic Control in the Ring Opening 3,3-Disubstituted 1,2-Dichlorocyclopropenes.
J. Chem. Soc., Chemical Communications, Issue 18, 1992, pp. 1323-1325.
- **Rzepa, Henry S. et al.**
Aryl Group n-Facial Electrostatic Asymmetry as a Contributing Factor to Chiral Resolution on beta-Cyclodextrin HPLC Phases.
J. Chem. Soc., Chemical Communications, Issue 16, 1992, pp. 1122-1124.
- **Rzepa, Henry S. et al.**
Crystallographic and PM3-COSMO SCF-MO Study of the Structure and Properties of Aryloxy- or Arylthio-thiazinones.
J. Chem. Soc., Perkin Transaction 2, 1994, pp. 185-188.
- **Rzepa, Henry S. et al.**
Electronic Effects in n-Facially Stereoselective Epoxidation of Phenyltrifluoromethylpropenol.
J. Chem. Soc., Chemical Communications, Issue 17, 1993, pp. 1337-1340.
- **Rzepa, Henry S. et al.**
Electrostatic vs. Orbital Control in n-Facial Diastereoselection: A PM3 SCF-MO Study of Electrophilic Reactivity in 7-Methylenenorbornanes.
Chem. Soc., Chemical Communications, Issue 14, 1992, pp. 998-1000.
- **Rzepa, Henry S. et al.**
n-Facial Hydrogen Bonding in the Chiral Resolving Agent (S)-2,2,2-Trifluoro-1-(9-anthryl)ethanol and its Racemic Modification.
J. Chem. Soc., Chemical Communications, Issue 11, 1991, pp. 765-768.
- **Rzepa, Henry S. et al.**
Origins of the Regioselectivity of Cyclopropylcarbonyl Ring Opening Reactions in Bicyclo [n.1.0] Systems.
J. Chem. Soc., Chemical Communications, Issue 13, 1992, pp. 942-944.
- **Rzepa, Henry S. et al.**
Selective n-Facial Binging of Metal Cations to Triindenotriphenylene as a Possible Catalytic Route to C60 Precursors: a MNDO, PM3 and ab initio SCF-MO Study.
J. Chem. Soc., Perkin Transaction 2, Issue 3, 1994, pp.
- **Rzepa, Henry S. et al.**
Stereoelectronic Influence of Fluorine in Enzyme Resolutions of alpha-Fluoroesters.
J. Chem. Soc., Perkin Transaction 2, Issue 1, 1994, pp. 3-4.
- **Rzepa, Henry S. et al.**
Theoretical Study of the Solvatochromic Properties of Rhodamines using the AM1 and PM3/COSMO Solvation Model.
J. Chem. Soc., Perkin Transaction 2, Issue 7, 1994, pp. 1397-1398.
- **Rzepa, Henry S. et al.,**
An SCF-MO Study of the Dimerisation Reaction of Hemifullerene (C30H12) to the Potential Fullerene Precursor C60H24.
J. Chem. Soc., Chem. Communication 2, 1994, pp. 1567-1568.
- **Rzepa, Henry S. et al.,**
Hyperactive Molecules and the World-Wide-Web information System.
J. Chem. Soc., Perkin Transaction 2, 1995, pp. 7-11.

- **Rzepa, Henry S., et al.**
 pi Facial Hydrogen Bonding in the Chiral Resolving Agent (S)-2,2,2-Trifluoro-1-(9-anthryl)ethanol and its Racemic Modification.
J. Chem. Soc., Chemical Communications, Issue 11, 1991, pp. 765-768.
- **S. Blumstengel, S. Sadofev, C. Xu, J. Puls, R. L. Johnson, H. Glowatzki, N. Koch, and F. Henneberger**
 Electronic coupling in organic-inorganic semiconductor hybrid structures with type-II energy level alignment
Phys. Rev. B 77, 085323 (2008)
- **S. V. Kessar, A. K. S. Mankotia, J. C. Scaiano, M. Barra's J. Gebicki, and K. Huben**
 Photochemistry of o-Vinylbenzaldehyde: Formation of a Ketene Methide Intermediate and Its Trapping with Secondary Amines
J. Am. Chem. Soc. 1996, 118(18), 4361-4365.
- **Sabat, Michael et al.**
 Potential Photoaffinity Labels for Tubulin. Synthesis and Evaluation of Diazocyclohexadienone and Azide Analogs of Colchicine, Combretastatin, and 3,4,5-Trimethoxybiphenyl.
J. Org. Chem., 59, 1994, pp. 4285-4296.
- **Salomon R. Billeter, Alessandro Curioni, Dominik Fischer, and Wanda Andreoni**
 Ab initio derived augmented Tersoff potential for silicon oxynitride compounds and their interfaces with silicon
Phys. Rev. B 73, 155329 (2006)
- **Sarah L. Hinchley, Carole A. Morrison, David W. H. Rankin, Charles L. B. Macdonald, Robert J. Wiacek, Andreas Voigt, Alan H. Cowley, Michael F. Lappert, Grete Gundersen, Jason A. C. Clyburne, and Philip P. Power**
 Spontaneous Generation of Stable Pnictinyl Radicals from "Jack-in-the-Box" Dipnictines: A Solid-State, Gas-Phase, and Theoretical Investigation of the Origins of Steric Stabilization
Journal of the American Chemical Society; 2001,123, 9045-9053.
- **Scheila F. Braga, Louraine C. de Melo, P.M.V.B. Barone**
 Semiempirical study on the electronic structure of antitumor drugs ellipticines, olivacines and isoellipticines
Journal of Molecular Structure: THEOCHEM, Volume 710, Issues 1-3, 26 November 2004, Pages 51-59
- **Schmiedekamp, Ann M. et al.**
 Theoretical Investigation of Reaction Pathways of 3-Methyloxadiazolinium Ion and 1,2,3-Oxadiazoline: Correlation with Experimental Findings.
J. Org. Chem., 59, 1994, pp. 3301-3306.
- **Schoch, Thomas K., S.D. Orth., M.C. Zerner, K.A. Jorgensen, L. McElwee-White,**
 Formation of Olefins Upon Oxidation of Molybdenum Alkyl Carbydes. Organic Radical Reactivity in an Organometallic Radical Cation.
Journal of the American Chemical Society, Vol. 117, No. 24, 1995, pp. 6475-6482.
- **Shih-Sheng Sun and Alistair J. Lees,**
 Self-Assembly Triangular and Square Rhenium(I) Tricarbonyl Complexes: A Comprehensive Study of Their Preparation, Electrochemistry, Photophysics, Photochemistry, and Host-Guest Properties
Journal of the American Chemical Society; 2000,122, 8956-8967.
- **Shinobu Itoh, Hideyuki Kumei, Shigenori Nagatomo, Teizo Kitagawa, and Shunichi Fukuzumi**
 Effects of Metal Ions on Physicochemical Properties and Redox Reactivity of Phenolates and

Phenoxy Radicals: Mechanistic Insight into Hydrogen Atom Abstraction by Phenoxy Radical-Metal Complexes

Journal of the American Chemical Society; 2001,123, 2165-2175.

- **Simon Jones, Chaiwat Smanmoo**
N-Phosphoryl oxazolidinones as effective phosphorylating agents
Tetrahedron Letters, Volume 45, Issue 8, 16 February 2004, Pages 1585-1588
- **Slater, Jonathan M. and J. Paynter and E.J. Watt.**
Multi-layer Conducting Polymer Gas Sensor Arrays for Olfactory Sensing.
Analyst, Vol. 118, April 1993, pp. 379-384.
- **Soghomonian, Victoria, et al.**
An Inorganic Double Helix: Hydrothermal Synthesis, Structure, and Magnetism of Chiral [(CH₃)₂NH₂]₄[V₁₀O₁₀(H₂O)₂(OH)₄(PO₄)₇]₄H₂O.
Science, Vol. 259, March 12, 1993, pp. 1596-1599, Cover.
- **Sonsoles Martin-Santamaria, Balasundaram Lavan and Henry S. Rzepa**
Huckel and Mobius aromaticity and trimerous transition state behaviour in the pericyclic reactions of [10], [14], [16] and [18]annulene
J. Chem. Soc., Perkin Trans. 2, 2000, 1415-1417. Received (in Cambridge, UK) 14th March 2000, Accepted 13th April 2000 Published on the Web 1st June 2000.
- **Sonsoles Martin-Santamaria, a Michael A. Carroll, a Victor W. Pike, b Henry S. Rzepa and David A. Widdowson**
An ab initio and MNDO-d SCF-MO computational study of the extrusion reactions of R₂ I-F iodine(III) via dimeric, trimeric and tetrameric transition state
J. Chem. Soc., Perkin Trans. 2, 2000, 2158-2161. Received (in Cambridge, UK) 17th January 2000, Accepted 7th July 2000 Published on the Web 24th August 2000.
- **Spressard, Gary O., et al.,**
Phytoalexin-like Activity of Abietic Acid and Its Derivatives
Journal of Agricultural and Food Chemistry, Vol. 43, No. 6, 1995, pp. 1690-1694.
- **Staempfli, Andreas and Zhongrui Zhou and July A. Leary.**
Gas-Phased Dissociation Mechanisms of Dilithiated Disaccharides: Tandem Mass Spectrometry and Semiempirical Calculations.
J. Org. Chem., Vol. 57, 1992, pp. 3590-3594.
- **Stanislaw Krompiec, Mariola Pigulla, Tadeusz Bieg, Wojciech Szczepankiewicz, Nikodem Kunik, Michal Krompiec, Maciej Kubicki**
Isomerisation of N-allyl-N-arylethanamides catalysed by ruthenium complexes
Journal of Molecular Catalysis A: Chemical, Volume 189, Issue 2, 24 October 2002, Pages 169-185
- **Steven M. LeCours, Stephen G. DiMugno, and Michael J. Therien**
Exceptional Electronic Modulation of Porphyrins through meso -Arylethynyl Groups. Electronic Spectroscopy, Electronic Structure, and Electrochemistry of [5,15-Bis[(aryl)ethynyl]-10,20-diphenylporphinato]zinc(II) Complexes. X-ray Crystal Structures of [5,15-Bis[(4'-fluorophenyl)ethynyl]-10,20-diphenylporphinato]zinc(II) and 5,15-Bis[(4'-methoxyphenyl)ethynyl]-10,20-diphenylporphyrin
J. Am. Chem. Soc. 1996, 118(47), 11854-11864.
- **Steven P. Keizer, John Mack, Barbara A. Bench, Sergiu M. Gorun, and Martin J. Stillman**
Spectroscopy and Electronic Structure of Electron Deficient Zinc Phthalocyanines
Journal of American Chemical Society; 2003, 125, 7067-7085
- **Suban K. Sahoo, Minati Baral, B.K. Kanungo**
Potentiometric, spectrophotometric, theoretical studies and binding properties of a novel

tripodal polycatechol-amine ligand with lanthanide(III) ions

Polyhedron, Volume 25, Issue 3, 13 February 2006, Pages 722-736

- **Suban K. Sahoo, Rati Kanta Bera, Minati Baral, B.K. Kanungo**
Excited state intramolecular proton transfer (ESIPT) in a dioxotetraamine derived schiff base and its complexation with Fe(III) and Cr(III)
Journal of Photochemistry and Photobiology A: Chemistry, Volume 188, Issues 2-3, 20 May 2007, Pages 298-310
- **Suban K. Sahoo, S.E. Muthu, Minati Baral, B.K. Kanungo**
Potentiometric and spectrophotometric study of a new dipodal ligand N,N'-bis{2-[(2-hydroxybenzylidene)amino]ethyl}malonamide with Co(II), Ni(II), Cu(II) and Zn(II)
Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, Volume 63, Issue 3, March 2006, Pages 574-586
- **Subhendu Mukherjee, Shuchi Nagar, Sanchita Mullick, Arup Mukherjee, Achintya Saha**
Pharmacophore mapping of arylbenzothiophene derivatives for MCF cell inhibition using classical and 3D space modeling approaches
Journal of Molecular Graphics and Modelling, Volume 26, Issue 5, January 2008, Pages 884-892
- **Sullivan CJ & CF Cooper.,**
Polyester weatherability: Coupling frontier molecular orbital calculations of oxidative stability with accelerated testing.
J. Coating Tech. Aug 1995.
- **Taber, Douglas F., J.P. Louey, Y. Wang, W.A. Nugent, D.A. Dixon, R.L. Harlow**
Stereoselectivity in Intramolecular Diene Cyclozirconation: A Combined Experimental and Theoretical Approach.
J. of the American Chemical Society, Vol. 116, No. 21, 1994, pp. 9457-9463.
- **Takai-T Senda-H Lee-HH Kuwae-A Hanai-K Kanazawa University**
We have identified for the first time symmetry allowed pathways for rearrangement of both the syn (1) and anti (2) isomers of the cyclobutadiene dimer in the closed shell potential energy surface for the isomerisation to cyclooctatetraene. At the B3LYP/6-31G(d) level of theory, the calculated activation energy for the reaction of 1 is 3.2 kcal mol⁻¹ lower than that for 2, in good agreement with the experimental difference of 3.6 kcal mol⁻¹. The possible influence of the sigma strain on the synchronicity of the pericyclic reactions of the systems is discussed. Keto-Enol-Tautomerism of Monosubstituted Phenylpyruvic Acids as Studied by NMR and PM3 Calculation
Spectroscopy Letters, 1998, 31, 2, p 379-95.
- **Teodozja Lipinska**
Experimental and theoretical FMO interaction studies of the Diels–Alder reaction of 5-acetyl-3-methylthio-1,2,4-triazine with cyclic enamines
Tetrahedron, Volume 61, Issue 34, 22 August 2005, Pages 8148-8158
- **Teresa Łuczak, Radosław Pankiewicz, Bogusława Łęska, Grzegorz Schroeder, Maria Bełtowska-Brzezinska, Bogumil Brzezinski**
Structure and electrochemical behaviour of 4,7-diazaheptyl-trimethoxy-silane and vinyl-trialkoxysilane adsorbed at silver surface
Journal of Molecular Structure, Volume 800, Issues 1-3, 4 December 2006, Pages 140-145
- **Thomson, Colin and Marshall Cory and Michael Zerner**
Theoretical Studies of Some New Anti-Malarial Drugs.
International Journal of Quantum Chemistry: Quantum Biology Symposium 18, 1991, pp. 231-245.

- **Tohru Fukuyama and Gang Liu**
Stereocontrolled Total Synthesis of (+/-)-Gelsemine
J. Am. Chem. Soc. 1996, 118(31), 7426-7427.
- **Toshihiko Hanai**
Simulation of chromatography of phenolic compounds with a computational chemical method
Journal of Chromatography A, Volume 1027, Issues 1-2, 20 February 2004, Pages 279-287
- **Toshio Hihara, Yasuyo Okada, Zenzo Morita**
A semiempirical molecular orbital study of the photo-reactivity of monoazo reactive dyes derived from 7- and 8-acids
Dyes and Pigments, Volume 73, Issue 2, 2007, Pages 141-161
- **Toshio Hihara, Yasuyo Okada, Zenzo Morita**
An analysis of the photo-reactivity of monoazo reactive dyes derived from 8-acid and related naphthalene sulfonic acids using the PM5 method
Dyes and Pigments, Volume 75, Issue 3, 2007, Pages 585-605
- **Toshio Hihara, Yasuyo Okada, Zenzo Morita**
Photo-oxidation of pyrazolinylazo dyes and analysis of reactivity as azo and hydrazone tautomers using semiempirical molecular orbital PM5 method
Dyes and Pigments, Volume 69, Issue 3, 2006, Pages 151-176
- **Toshio Hihara, Yasuyo Okada, Zenzo Morita**
Reactivity of phenylazonaphthol sulfonates, their estimation by semiempirical molecular orbital PM5 method, and the relation between their reactivity and azo-hydrazone tautomerism
Dyes and Pigments, Volume 59, Issue 3, December 2003, Pages 201-222
- **Toshio Hihara, Yasuyo Okada, Zenzo Morita**
The photo-oxidation of reactive azobenzene dyes and an analysis of their reactivity for the azo and hydrazone tautomers using the semiempirical molecular orbital PM5 method
Dyes and Pigments, Volume 75, Issue 1, 2007, Pages 225-245
- **Trost, Barry M., Thomas J. J. Muller, and Jose Martinez,**
Ruthenium-Catalyzed Synthesis of Butenolides and Pentenolides via Contra-Electronic α -Alkylation of Hydroxyalkynoates
J. Am. Chem. Soc. 1995, 117, 1888-1899.
- **Turchi, Ignatius J. and Cynthia A. Maryanoff**
Mechanism and Stereochemical Implications of the Reaction of Oxazolium-5-Oxide with 1,2-Dicyanocyclobutene. An AM1 Study.
Heterocycles, Vol. 35 No. 2, 1993, pp. 649-657.
- **Turchi, Ignatius J. et al.**
Interesting Contrasts in Electrocyclic Reactions for Thieno[3,2-b]- and -[3,2-b]pyrans with Chromenes.
J. Org. Chem., 58, 1993, pp. 4629-4633.
- **van der Linden, Arjan, Colin J. Schaverien, Nico Meijboom, Christian Ganter, and A. Guy Orpen,**
Polymerization of α -Olefins and Butadiene and Catalytic Cyclotrimerization of 1-Alkynes by a New Class of Group IV Catalysts
J. Am. Chem. Soc. 1995, 117, 3008-3021.
- **Wegner, Peter J., Bong-Ser Park, Martin Sobczak, Joseph Frey, and Zvi Rappoport,**
Photocyclization of 2,4,6,2',4',6' Hexaalkylbenzils
J. Am. Chem. Soc. 1995, 117, 7619-7629.

- **Weijin Li and Marye Anne Fox**
Syntheses, Characterization, and Photophysics Studies of Photoactive Chromophore 2-Naphthyl-Labeled [n]-Ladderanes
J. Am. Chem. Soc. 1996, 118(47), 11752-11758.
- **West, Jon K. and Larry L. Hench**
Silica fracture - Part I. A ring contraction model.
Journal of Materials Science, Vol., 29, 1994, pp. 3601-3606.
- **West, Jon K. and Larry L. Hench**
Silica fracture - Part II. A ring opening model via hydrolysis.
Journal of Materials Science, Vol. 29, 1994, pp. 5808-5816.
- **West, Jon K. and Larry L. Hench,**
Inorganic pathways for biosynthesis: A molecular orbital modeling approach.
J. Vac. Sci. Technology A Vol. 12, No. 5, 1994, pp. 2962-2965.
- **West, Jon K. and Larry L. Hench,**
Molecular Orbital Models of Silica Rings and Their Vibrational Spectra.
J. of American Ceramic Soc., Vol. 78, No. 4, 1995, pp. 1093-1096.
- **West, Jon K. and Larry L. Hench,**
Molecular Orbital Models of Silica.
Annu. Rev. Mater. Sci., Vol. 25, 1995, pp. 37-68.
- **West-JK Brennan-AB Clark-AE Zamora-M Hench-LL**
Cyclic Anhydride Ring-Opening Reactions - Theory and Application
Journal of Biomedical Materials Research 1998, Vol 41, Iss 1, pp 8-17.
- **Wong, Chi-Huey, et al.**
Sugar Nucleotide recycling
J. Am. Chemical Society, 114, 9283 (1992).
- **Xiang Li, Jie Wang, Richard Mason, Xiu R. Bu, Joycelyn Harrison**
Combined phase transfer catalysis and ultrasound to enhance tandem alkylation of azo dyes
Tetrahedron, Volume 58, Issue 19, 6 May 2002, Pages 3747-3753
- **Xiankai Sun, Darren W. Johnson, Dana L. Caulder, Kenneth N. Raymond, and Edward H. Wong**
Rational Design and Assembly of M₂M'₃L₆ Supramolecular Clusters with C_{3h} Symmetry by Exploiting Incommensurate Symmetry Numbers
Journal of the American Chemical Society, 2001,123, 2752-2763.
- **Yasuhiro Shigemitsu, Kaori Komiya, Naoko Mizuyama, Yoshinori Tominaga**
Reaction of functionalized maleimides with versatile nucleophiles. Synthesis, electronic spectra and molecular orbital study
Dyes and Pigments, Volume 72, Issue 3, 2007, Pages 271-284
- **Yasuyo Okada, Toshio Hihara, Zenzo Morita**
Analysis of the catalytic fading of pyridone-azo disperse dyes on polyester using the semi-empirical, molecular orbital PM5 method
Dyes and Pigments, Volume 78, Issue 3, September 2008, Pages 179-198
- **Yasuyo Okada, Toshio Hihara, Zenzo Morita**
Analysis of the photofading of phenylazo-aniline and phenylazo-pyridone disperse dyes on poly(ethylene terephthalate) substrate using the semiempirical molecular orbital PM5 method
Dyes and Pigments, Volume 79, Issue 2, November 2008, Pages 111-125
- **Young Soo Keum, Qing X. Li**
Fungal laccase-catalyzed degradation of hydroxy polychlorinated biphenyls
Chemosphere, Volume 56, Issue 1, July 2004, Pages 23-30

- **Yukitami Mizuno, Takuzo Aida, and Kentaro Yamaguchi,**
Chirality-Memory Molecule: Crystallographic and Spectroscopic Studies on Dynamic Molecular Recognition Events by Fully Substituted Chiral Porphyrins
Journal of the American Chemical Society; 2000,122, 5278-5285.
- **Zhiguang Xiao, Robert W. Gable, Anthony G. Wedd, and Charles G. Young,**
Complexes Containing cis- [MoV O₂] + and cis-[MoV O(OH)]₂⁺ Centers
J. Am. Chem. Soc. 1996, 118(12), 2912-2921.

Materials Explorer publications:

- **A. Honda, K. Matsunaga and H. Matsubara**
Molecular Dynamics Simulation of an Intergranular Glass Phase in Alumina Based Ceramics
J. Japan Inst. Metals, Vol. 64, No. 11(2000),pp. 1113-1119
- **A. Takeuchi, K. Yubuta, Y. Yokoyama, A. Makino, A. Inoue**
Noncrystalline atomic arrangements computationally created from crystalline compound by treating groups of atoms as hypothetical clusters
Intermetallics, Volume 16, Issue 2, February 2008, Pages 283-292
- **A. Takeuchi, K. Yubuta, Y. Yokoyama, A.R. Yavari, A. Inoue**
Noncrystalline structure created through ensemble of clusters in metastable cubic Zr₂Ni structure by their random rotations and subsequent annealing
Intermetallics, Volume 16, Issue 6, June 2008, Pages 774-778
- **A. Takeuchi, Y. Yokoyama, H. Kato, K. Yubuta, A. Inoue**
Formation of Zr_{66.7}Al_{11.1}Ni_{22.2} noncrystalline alloys demonstrated by molecular dynamics simulations based on distorted plastic crystal model
Intermetallics, Volume 16, Issue 6, June 2008, Pages 819-826
- **Alistair P. Rendell, Andrey Bliznyuk, Thomas Huber, Ross H. Nobes, Elena V. Akhmatskaya, Herbert A. Fruchtl, Paul W. -C. Kung, Victor Milman, Han Lung**
Computational chemistry on Fujitsu vector-parallel processors: Development and performance of applications software
Parallel Computing, Volume 26, Issues 7-8, July 2000, Pages 887-911
- **C.A.J. Fisher, M. Yoshiya, Y. Iwamoto, J. Ishii, M. Asanuma, K. Yabuta**
Oxide ion diffusion in perovskite-structured Ba_{1-x}Sr_xCo_{1-y}FeyO_{2.5}: A molecular dynamics study
Solid State Ionics, Volume 177, Issues 39-40, 15 January 2007, Pages 3425-3431
- **Ephraim Bulemela, Peter Tremaine, Shun-ichi Ikawa**
Volumetric behavior of water-methanol mixtures in the vicinity of the critical region
Fluid Phase Equilibria, Volume 245, Issue 2, 10 August 2006, Pages 125-133
- **Fujii, K.; Soejima, Y.; Kyoshoin, Y.; Fukuda, S.; Kanzaki, R.; Umebayashi, Y.; Yamaguchi, T.; Ishiguro, S.-i.; Takamuku, T.**
Liquid Structure of Room-Temperature Ionic Liquid, 1-Ethyl-3-methylimidazolium Bis-(trifluoromethanesulfonyl) Imide
J. Phys. Chem. B.; (Article); 2008; 112(14); 4329-4336. DOI: 10.1021/jp7105499
- **Fumio Tanaka, Somchai Keawwangchai, Rong Rujkorakarn, Noboru Mataga**
Study of photo-induced electron transfer in pyrene-(CH₂)_n-N,N'-dimethylaniline system by molecular dynamic simulation
Chemical Physics, Volume 348, Issues 1-3, 2 June 2008, Pages 242-248

- **H. Suzuki, H. Matsubara, J. Kishino and T. Kondoh**
Simulation of Surface and Grain Boundary Properties of Alimina by Molecular Dynamics Method
Journal of the Ceramic Society of Japan, 106[12], 1215-1222(1998)
- **H. Toriumi, M. Yoshida, M. Mikami, M. Takeuchi and A. Mochizuki**
Computer Simuration of an Antiferroelectric Liquid Crystalline Molecule: The Origin of Bent Structure Formation and the Molecular Packing Property of MHPOBC in Crystalline Phase
J. Phys. Chem., Vol. 100, No. 37(1996)
- **H. Toriumi, M. Yoshida, N. Kamiya and M. Takeuchi**
Molecular Dynamics Simulation of an Antiferroelectric Liquid Crystalline Molecule MHPOBC: Conformational Transition in Smectic Phases
Mol. Cryst. Liq. Cryst., Vol. 402, pp. 31/[267]-42/[278],(2003)
- **Hesske, H.; Gloe, K.**
Hydration Behavior of Alkyl Amines and Their Corresponding Protonated Forms. 1. Ammonia and Methylamine
J. Phys. Chem. A.; (Article); 2007; 111(39); 9848-9853. DOI: 10.1021/jp073154a
- **Hideaki Matsubara**
Computer simulations for the design of microstructural developments in ceramics
Computational Materials Science, Volume 14, Issues 1-4, February 1999, Pages 125-128
- **K. Matsunaga and H. Matsubara**
Molecular Orbital Calculations on Atomic Structures of Si-Based Covalent Amorphous Ceramics
Mat. Res. Soc. Symp. Proc. Vol. 538(1999)Materials Research Society
- **K. Matsunaga, C. Fisher and H. Matsubara**
Tersoff Potential Parameters for Simulating Cubic Boron Carbonitrides
Jpn. J. Appl. Phys. Vol. 39(2000), pp. L48-51
- **K. Matsunaga, S. Ii, C. Iwamoto, T. Yamamoto and Y. Ikuhara**
In situ observation of crack propagation in magnesium oxide ceramics
Nanotechnology 15(2004)S376-S381
- **K. Matsunaga, Y. Iwamoto, C. A. J. Fisher and H. Matsubara**
Molecular Dynamics Study of Atomic Structures in Amorphous Si-C-N Ceramics
Journal of the Ceramic Society of Japan, 107[11], 1025-1031(1999)
- **M. Nakamura, H. Fujioka, K. Ono, M. Takeuchi, T. Mitsui, M. Oshima**
Molecular dynamics simulation of III-V compound semiconductor growth with MBE
Journal of Crystal Growth, Volume 209, Issues 2-3, February 2000, Pages 232-236
- **M. Takahashi, T. Maeda, K. Sakiyama, H. Takano, M. Itoh**
Molecular dynamic simulation on the cool-liquefaction of nano-cluster by quantum size effect
Journal of Aerosol Science, Volume 31, Supplement 1, September 2000, Pages 915-916
- **M. Takeuchi, Y. Masuda and S. Muto**
Classical Molecular Dynamics Method As A Tool For Studying Phase Transformations; Proceedings of the International Conference on Solid-Solid Phase Transformations '99(JIMIC-3) Edited by M. Koiwa, K. Otsuka and T. Miyazaki
The Japan Institute of Metals, 1999.
- **M. Yoshiya, et al.**
Perturbed Molecular Dynamics for Calculating Thermal Conductivity of Zirconia
Molecular Simulation Vol30(13-15) P953-961
- **Okobira, T.; Miyoshi, K.; Uezu, K.; Sakurai, K.; Shinkai, S.**
Molecular Dynamics Studies of Side Chain Effect on the β -1,3-D-Glucan Triple Helix in

Aqueous Solution

Biomacromolecules; (Article); 2008; 9(3); 783-788. DOI: 10.1021/bm700511d

- **R. Kojima, M. Susa**
Melting of thin γ -Fe-C films having (100), (110) and (111) surfaces in terms of molecular dynamics simulation
Science and Technology of Advanced Materials, Volume 5, Issues 5-6, September-November 2004, Pages 677-682
- **R. Kojima, M. Susa**
Second moment approximation of tight-binding potential for γ -Fe applicable up to 1700 K
Science and Technology of Advanced Materials, Volume 5, Issue 4, July 2004, Pages 497-502
- **R. Tarumi, A. Ogura, M. Shimojo, K. Takashima and Y. Higo**
Molecular Dynamics Simulation of Crystallization in an Amorphous Metal during Shear Deformation
Jpn. J. Appl. Phys. Vol. 39(2000)pp. L611-L613
- **Ross H. Nobes, Alistair P. Rendell, Jarek Nieplocha**
Computational chemistry on Fujitsu vector-parallel processors: Hardware and programming environment
Parallel Computing, Volume 26, Issues 7-8, July 2000, Pages 869-886
- **S. Ii, C. Iwamoto, K. Matsunaga, T. Yamamoto, Y. Ikuhara**
TEM in situ observation of fracture behavior in ceramic materials
Applied Surface Science, Volume 241, Issues 1-2, 28 February 2005, Pages 68-74
- **S. Muto, M. Takeuchi, Y. Masuda and T. Tanabe**
Local Atom Displacements Around Crystal Lattice Defects Inducing Phase Transformations Studied by Molecular Dynamics Simulation; The Third Pacific Rim International Conference on Advanced Materials and Processing (PRICM3) Edited by M. A. Imam, R. DeNale, S. Hanada, Z. Zhong and D. N. Lee
The Minerals, Metals & Materials Society, 1998
- **S. Muto, Y. Masuda and M. Takeuchi**
Molecular Dynamics Study on Local Atomic Displacements Associated with Point Defects and Displacive Phase Transformations
Materials Transactions, JIM, Vol. 40, No. 6(1999), pp. 514 to 521
- **Satoshi Kojima, Chao Hu**
Plastic deformation by synchronized rotation of nanolayers under high stress in metals
Materials Science and Engineering: A, In Press, Corrected Proof, Available online 6 January 2008
- **Shohei Arai, Manabu Togashi, Mariko Shiozawa, Yoshio Inoue, Minoru Sakurai**
Molecular dynamics simulation of the M intermediate of photoactive yellow protein in the crystalline state
Chemical Physics Letters, Volume 414, Issues 1-3, 3 October 2005, Pages 230-233
- **Shuhei Fukuda, Munetaka Takeuchi, Kenta Fujii, Ryo Kanzaki, Toshiyuki Takamuku, Kazumi Chiba, Hideo Yamamoto, Yasuhiro Umebayashi, Shin-ichi Ishiguro**
Liquid structure of N-butyl-N-methylpyrrolidinium bis-(trifluoromethanesulfonyl) amide ionic liquid studied by large angle X-ray scattering and molecular dynamics simulations
Journal of Molecular Liquids, In Press, Corrected Proof, Available online 21 March 2008
- **T. Kurobori, K. Inabe, S. Aoshima, T. Itoh, M. Takeuchi and E. Radzhabov**
Time-resolved study and molecular dynamics simulation of defect centers in BaFX (X=Cl, Br) crystals
Journal of Luminescence 87-89(2000)558-560

- **T. Kurobori, M. Liu, H. Tsunekawa, Y. Hirose and M. Takeuchi**
Molecular Dynamics Simulation of the Pressure-Induced Phase Transition In BaFCl
Radiation Effects & Defects in Solids, 2002, Vol. 157, pp. 799-803
- **T. Kurobori, M. Yoshiura, Min Liu and Y. Hirose**
Vacancy Migration Properties of BaFCl Obtained by Molecular Dynamics Simulation
Jpn. J. Appl. Phys. Vol. 38(1999)pp. L948-L950
- **T. Kurobori, S. Kozake, T. Kawamoto and Y. Hirose**
Thermal Properties of BaFCl Crystals Simulated by Molecular Dynamics
Jpn. J. Appl. Phys. Vol. 39(2000)pp. L537-L540, Part2, No. 6A(1 June 2000)
- **T. Kurobori, Y. Hirose and M. Takeuchi**
Thermal Expansion Coefficient of BaFX (X=Cl, Br) by Molecular Dynamics Simulation
Rapid Research Notes: 00-017(2000)
- **Takeo Oku, Masaki Kuno, Hidehiko Kitahara, Ichihito Narita**
Formation, atomic structures and properties of boron nitride and carbon nanocage fullerene materials
International Journal of Inorganic Materials, Volume 3, Issue 7, November 2001, Pages 597-612
- **W. C. Lie, A. S. Acosta, H. Fujioka, T. Mano, T. Mitsui, M. Takeuchi, M. Oshima**
Theoretical study of embedded InAs quantum dots in GaAs
Journal of Crystal Growth, Volume 229, Issues 1-4, July 2001, Pages 615-618
- **W.H. Qi, B.Y. Huang, M.P. Wang, F.X. Liu, Z.M. Yin**
Freezing of silver cluster and nanowire: A comparison study by molecular dynamics simulation
Computational Materials Science, Volume 42, Issue 3, May 2008, Pages 517-524
- **Xue-jun ZHENG, Bo YANG, Zhe ZHU, Bo WU, Yu-liang MAO**
Kinetic Monte Carlo simulation of growth of BaTiO₃ thin film via pulsed laser deposition
Transactions of Nonferrous Metals Society of China, Volume 17, Issue 6, December 2007, Pages 1441-1446
- **Y. Kameda, M. Imano, M. Takeuchi, S. Suzuki, T. Usuki, O. Uemura**
Neutron diffraction and MD studies of LiBr hydrated melts
Journal of Non-Crystalline Solids, Volumes 293-295, November 2001, Pages 600-606
- **Yoshikazu Suzuki, Tatsuki Ohji**
Anisotropic thermal expansion of calcium dialuminate (CaAl₄O₇) simulated by molecular dynamics
Ceramics International, Volume 30, Issue 1, 2004, Pages 57-61
- **Yunmin Yang, Hiroaki Abe, Naoto Sekimura**
Behavior of Frank-loops under stress environment
Physics Letters A, Volume 315, Issues 3-4, 25 August 2003, Pages 293-300
- **Yutaka Maniwa, Kazuyuki Matsuda, Haruka Kyakuno, Syunsuke Ogasawara, Toshihide Hibi, Hiroaki Kadowaki, Shinzo Suzuki, Yohji Achiba and Hiromichi Kataura**
Water-filled single-wall carbon nanotubes as molecular nanovalves
Nature Materials, Volume 6, Issue 2, February 2007, Pages 135-141
- **Zhi-qiang Li, K. Ohno, Y. Kawazoe, M. Mikami, Y. Masuda**
Energetics and structures of small benzene clusters
Z.-q. Li et al./Computational Materials Science 4(1995)241-248

The list includes publications from SCIGRESS and its predecessors CAChe and Materials Explorer.