

## Em. Prof. dr hab. Mirosław Szafran

Publikacje 2007

### 1.a. Publikacje w czasopismach wyróżnionych z listy Filadelfijskiego Instytutu Informacji Naukowej

1. „Synthesis, spectral and B3LYP analysis of 1-R-2-oxo-pyrido[2,1b][3,4]dihydro-pyrimidinium halides”  
I.Kowalczyk, M.Szafran  
ARKIVOC vi, 2007, p.55-63
2. „Crystal and molecular structure of 4-carboxypiperidinium chloride (4-piperidinecarboxylic acid hydrochloride)”  
M.Szafran, A.Komasa, E.Bartoszak-Adamska  
J. Mol. Struct. 827, 2007, p.101-107
3. „Crystal and molecular structure, hydrogen bonding and electrostatic interactions of bis(homarine) hydrogen perchlorate studied by X-ray diffraction, DFT calculations, FTIR and Raman spectroscopies”  
M.Szafran, A.Katrusiak, Z.Dega-Szafran  
J. Mol. Struct. 839, 2007, p.99-106
4. „Hydrogen bonds and electrostatic interactions in 1:1 and 2:1 complexes of homarine with mineral acids studied by NMR, FTIR, DFT and X-ray diffraction”  
M.Szafran, A.Katrusiak, Z.Dega-Szafran  
J. Mol. Struct. 827, 2007, p.56-66
5. „Molecular structure and spectroscopic properties of the complex of N-methylmorpholine betaine with 3,4-dinitrophenol”  
Z.Dega-Szafran, A.Katrusiak, M.Szafran  
J. Mol. Struct. 841, 2007, p.125-132
6. „Molecular structure, hydrogen bonding, basicity and spectroscopic properties of 3-hydroxypyridine betaine hydrochloride monohydrate”  
P.Barczyński, A.Komasa, A.Katrusiak, Z.Dega-Szafran, M.Szafran  
J. Mol. Struct. 832, 2007, p.63-72
7. „Structure of 1-methyl-2-oxo-pyrido[2,1b][3,4]dihydropyrimidinium bromide studied by X-ray diffraction, FTIR and NMR spectroscopy and DFT calculations”  
M.Szafran, I.Kowalczyk, E.Bartoszak-Adamska, M.Jaskólski, B.Nowak-Wydra  
J. Mol. Struct. 843, 2007, p.107-115
8. „Structure of 1-methylpyridinium-4-carboxylate monohydrate studied by X-ray, FT-IR, Raman, NMR and ab initio methods”  
M.Szafran, E.Bartoszak-Adamska, J.Koput, Z.Dega-Szafran  
J. Mol. Struct. 844-845, 2007, p.140-156
9. „Structure of the 2:1 complex of 1-piperidineacetic acid and p-hydroxybenzoic acid studied by X-ray, FTIR, 1H, 13C NMR, and DFT methods”  
Z.Dega-Szafran, G.Dutkiewicz, Z.Kosturkiewicz, M.Szafran  
J. Mol. Struct. 844-845, 2007, p.38-47
10. „Structure, conformation and hydrogen bonding of 4-(N-methylpiperidinium)-butyric acid bromide”  
Z.Dega-Szafran, E.Dulewicz, M.Szafran, R.Thaimattam, M.Jaskólski  
J. Mol. Struct. 828, 2007, p.19-24
11. „X-ray and ab initio studies of the structure, vibrational and NMR spectra of 1-methyl-3-hydroxypyridinium chloride”  
M.Szafran, A.Komasa, A. Katrusiak, Z.Dega-Szafran, P.Barczyński  
J. Mol. Struct. 844-845, 2007, p.102-114
12. „X-ray, MP2 and DFT studies of the structure, vibrational and NMR spectra of homarine”  
M.Szafran, A.Katrusiak, J.Koput, Z.Dega-Szafran  
J. Mol. Struct. 846, 2007, p.1-12
13. „Crystal and Molecular Structure of 1:1 Complex Between Piperidine-3-carboxylic Acid and p-Hydroxybenzoic Acid Studied by X-ray Diffraction, FTIR, 1H and 13C NMR Spectroscopy, and B3LYP Method”  
Z.Dega-Szafran, M.Jaskólski, M.Szafran  
Pol. J. Chem. 81, 2007, p.931-946

### 1.c. Publikacje w recenzowanych wydawnictwach zbiorowych

1. „Structure of the complex of piperidineacetic acid with p-hydroxybenzoic acid and related compounds” w "Annals of Polish Chemical Society'2007"  
Z.Dega-Szafran, G.Dutkiewicz, Z.Kosturkiewicz, M.Szafran  
PTCh Gdańsk, 2007, p.103-106

Dane wg. stanu na dzień 8.04.2008

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2. „DFT Calculation of structure and vibrational spectrum of  $\beta$ -4-hydroxy-1-methyl-piperidine betaine hydrochloride" w "Annals of Polish Chemical Society'2007"

M.Szafran, Z.Dega-Szafran, J.Koput, E.Dulewicz, W.B.Person, K.Szczepaniak  
PTChem Gdańsk , 2007, p.573-576

### **2.b.2. Autorstwo rozdziału w monografii lub podręczniku akademickim w języku polskim lub innym nie angielskim**

1. „Betainy i ich kompleksy z kwasami" w "Na pograniczu chemii i biologii"

M.Szafran, Z. Dega-Szafran  
Wyd. Naukowe UAM XVIII, 2007, p.255-275