

Em. Prof. dr hab. Zofia Dega-Szafran

Publikacje 2006

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

1. „Cocrystals of bis(4-hydroxy-1-methylpiperidine betaine) hydrochloride”
Z.Dega-Szafran, E.Dulewicz, G.Dutkiewicz, Z.Kosturkiewicz
J. Mol. Struct. 794, 2006, p.54-62
2. „Conformational analysis of bis(trigonelline) hydrochloride, perchlorate and their monohydrates by the B3LYP calculations, X-ray diffraction and vibrational spectra”
M.Szafran, A.Katrusiak, J. Koput, Z.Dega-Szafran
J. Mol. Struct. 784, 2006, p.98-108
3. „Hydrogen bonds and conformational analysis of bis(1-methylisonicotinate) hydrochloride monohydrate by X-ray diffraction, vibrational spectra and B3LYP calculations”
M.Szafran, A.Katrusiak, Z.Dega-Szafran
J. Mol. Struct. 794, 2006, p.46-53
4. „NMR study of 4-hydroxy-1-methylpiperidine betaine derivatives”
Z.Dega-Szafran, E.Dulewicz, M.Szafran
J. Mol. Struct. 792-793, 2006, p.50-55
5. „Structure and properties of the 1:2 complex of 1,4-dicarboxymethyl-1,4-dimethylpiperazinium inner salt (di-betaine) with p-hydroxybenzoic acid studied by X-ray, DFT, FTIR and NMR methods”
Z.Dega-Szafran, A.Katrusiak, M.Szafran
J. Mol. Struct. 797, 2006, p.82-91
6. „Structure of 3-hydroxy-3-phenyl-pyrido[2,1-c][1,4]dihydrooxazinium bromide studied by X-ray, FTIR, 1H, 13C and 15N NMR, and DFT methods”
M.Szafran, B.Nowak-Wydra, A.Katrusiak, Z.Dega-Szafran
J. Mol. Struct. 792-793, 2006, p.36-49
7. „X-ray and ab initio studies of the structure and vibrational spectra of 4-carboxy-1-methylpyridinium chloride”
M.Szafran, J.Koput, Z.Dega-Szafran, A.Katrusiak
J. Mol. Struct. 797, 2006, p.66-81
8. „X-ray, NMR and DFT studies of the complex of 1,4-dimethylpiperazine mono-betaine with p-hydroxybenzoic acid”
Z.Dega-Szafran, A.Katrusiak, M.Szafran
J. Mol. Struct. 785, 2006, p.160-166
9. „Structure of 3-Hydroxy-3-methyl-pyrido[2,1-c][1,4]dihydrooxazinium Chloride Studied by X-ray, FTIR, 1H, 13C and 15N NMR and DFT Methods”
M.Szafran, B.Nowak-Wydra, A.Katrusiak, Z.Dega-Szafran
Pol. J. Chem. 80, 2006, p.1039-1053

1.b. Publikacje w innych recenzowanych czasopismach nie będących na liście Filadelfijskiej o cyrkulacji międzynarodowej

1. „DFT calculation of structure and vibrational spectrum of 1-methylisonicotinic acid chloride”
M.Szafran, J.Koput, Z.Dega-Szafran
Asian J. Phys. 15(2), 2006, p.253-258