CHEMISTRY JOURNAL OF MOLDOVA. General, Industrial and Ecological Chemistry. 2016, 11(2), 58-67
http://cjm.asm.md
http://dx.doi.org/10.19261/cjm.2016.11(2).07

SYNTHESIS, SPECTRAL AND THEORETICAL CHARACTERIZATION OF 5,6-DICHLORO/DIMETHYL-2-(2´,3´/2´,4´/2´,5´/3´,4´/3´,5´-DIMETHOXYPHENYL)-1*H*-BENZIMIDAZOLES

Demet Gürbüz[a], Aydin Tavman[a*], Adem Cinarli[a], Ismail Boz[b]

[a]*Istanbul University, Faculty of Engineering, Department of Chemistry, 34320, Avcilar, Istanbul, Turkey*
[b]*Istanbul University, Faculty of Engineering, Department of Chemical Engineering, 34320, Avcilar, Istanbul, Turkey*
[*]*e-mail: atavman@istanbul.edu.tr; phone: (+90) 21 247 370 70; fax: (+90) 21 247 371 80*

Abstract. 5,6-Dichloro/dimethyl-2-(2´,3´/2´,4´/2´,5´/3´,4´/3´,5´-dimethoxyphenyl)-1*H*-benzimidazoles were synthesized and characterized by using analytical data, FT-IR, FT-Raman, NMR, ESI-MS and fluorescence spectroscopy. The optimized molecular geometry, zero point energy, dipole moment, ESE, band gap and charge distributions were calculated by Gaussian 09 using Density Functional Theory (DFT, RB3LYP) with 6-31++G(d,p) basis set. According to the calculations, the molecules have structures with various torsion angles between the benzimidazole and benzene rings from 9.7º to 47.8º. The calculated energy values with ZPE correction and DFT show that the methyl derivatives are more stable than the chloro forms. 3´,4´-Dimethoxy derivatives have higher decomposition points in comparison with the other compounds in series. The chlorine atoms of 5,6-dichloro-2-(2´,3´/2´,4´/2´,5´/3´,4´/3´,5´-dimethoxyphenyl)-1*H*-benzimidazoles are positively charged whereas the C5 and C6 carbon atoms are negatively charged due to the attached chlorine atoms, in virtue of the electron withdrawing characteristic of the imidazole part of the benzimidazole ring. Also, some calculated prominent bond lengths and bond angles were discussed.

Keywords: dimethoxyphenylbenzimidazoles, spectral characterization, density functional theory, charge distribution, geometry optimization.

Received: June 2016/ Revised final: November 2016/ Accepted: November 2016