DFT Calculation, Anion Sensing Application Studies and Crystal Structure of 3-Aminopyridine-Based Imine Derivative

B. Boyacioglu[1], H. Ünver[2], M. Yıldız[3] , C.T. Zeyrek[4] and A. Elmalı[5]

[1]Vocational School of Health Services, Ankara University, TR-06290 Kecioren-Ankara, Turkey
E-mail:bboyacioglu@ankara.edu.tr

[2]Department of Physics, Faculty of Sciences, Ankara University, TR-06100 Besevler-Ankara, Turkey

[3]Department of Chemistry, Faculty of Sciences and Arts, Çanakkale Onsekiz Mart University, TR-17100 Çanakkale, Turkey

[4]Ankara Nuclear Research and Training Center, Turkish Atomic Energy Authority, TR-06100 Ankara, Turkey

[5] Department of Physics Engineering, Faculty of Engineering, Ankara University, TR-06100, Beşevler , Turkey

The 3-aminopyridine-based imine derivative (*E*)-4-((pyridin-3-ylimino)-methyl)benzene-1,3-diol was synthesized from the reaction of 3-aminopyridine with 2,4-dihydroxybenzaldehyde. Characterization of the ligand was carried out using theoretical quantum-mechanical calculations and experimental spectroscopic methods. The molecular structure of the compound was confirmed using X-ray single-crystal data, NMR, FTIR and UV-Visible spectroscopy, which were in good agreement with the structure predicted by the theoretical calculations using density functional theory (DFT)[1-3].

The colorimetric response of the ligand in DMSO to the addition of equivalent amount of anions (F^-, Br^-, I^-, CN^-, SCN^-, ClO_4^-, HSO_4^-, AcO^-, $H_2PO_4^-$, N_3^- and OH^-) was investigated and the ligand was shown to be sensitive to F^-, CN^-, AcO^- and OH^- anions [4-5].

1. *K.S. Thanthiriwatte, K.M.N. de Silva*, J. Mol. Struc-Theochem, 2002, **617**, 169-175.
2. A.V. Marenich, C.J. Cramer, D.G. Truhlar, J. Phys. Chem. B. 2009, **113**, (18) 6378–6396
3. *C.T. Zeyrek, B. Boyacioğlu, M. Yıldız, H. Ünver, D. Yolal, N. Demir, A. Elmalı, S. Tadesse, K. Aslan*, Bioorganic & Medicinal Chemistry, 2016, **24**, 5592-5601.
4. *R. A, Badugu*, Sensors and Actuators B: Chemical 2005, **104**, 103-110.
5. *L.Yuan, W. Lin, Y. Yang, J. Song, J. Wang*, Org. Lett. 2011, **13**, 3730-37