Turkish Journal of Chemistry

Turkish Journal

of

Chemistry

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A Quantum-Chemical Investigation on 5,5'-Bi(1H-1.2,4-Triazole))

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Abstract: The conformational analysis of flexible 5,5'-bi(1H-1,2,4-triazole) molecule containing various reaction centers has been perform by the semiempirical methods MNDO,AM1 and PM3, and the internal rotation barrier calculated. The most stable conformation of the molecule has been determined to be the planar trans conformation. According to the three methods, 5,5'-bi(1H-1,2,4-triazole) molecule (C has been found to be relatively more stable than its tautomer 3,3'-bi(1H-1,2,4-triazole)(B) and to be less stable than its other tautomer 3,3 bi(4H-1,2,4-triazole)(A). Moreover, the electronic properties of 5,5'-bi(1H-1,2,4-triazole) molecule and the effect of conformational changing on electronic and geometric properties have also been investigated. To determine the protonation sites of the 5,5'- bitriazole system, the molecular electrostatic poential (MESP) of the molecule has been calculated. The electronic properties and conformations of the monoprotonated species formed from the protonation of the molecule have also been studied using AM1 and PM3 routes. The proton affinity of the 5,5'-bitriazole molecule has been calculated for the different nitrogens using AM1 and PM3 methods and the possible protonation centers have been determined. The electronic properties and the geometry of Fe^{2+} complex of the bitriazole system have bee investigated by ZINDO/1 method and its formation process has been searched theoretically. According to proton affinity values, the complex formation ability of A, B and C tautomers of bi(1,2,4-triazole) system have been evaluated and the stabilities of their Fe^{2+} complexes have been determined by ZINDO/1 route. It has been found that tautomer B has a higher complex formation ability and forms more stable metal complexes relative to the other tautomers. Keywords: 1,2,4-triazol, conformational analysis, protonation affinity, tautomerism, electronic properties.

Turk. J. Chem., **21**, (1997), 353-362.
Full text: pdf
Other articles published in the same issue: Turk. J. Chem.,vol.21,iss.4.