Vali-e-Asr University of Rafsanjan

19th Iranian Seminar on Organic Chemistry
Vali-e-Asr University of Rafsanjan, 5 -7 Sep. 2012

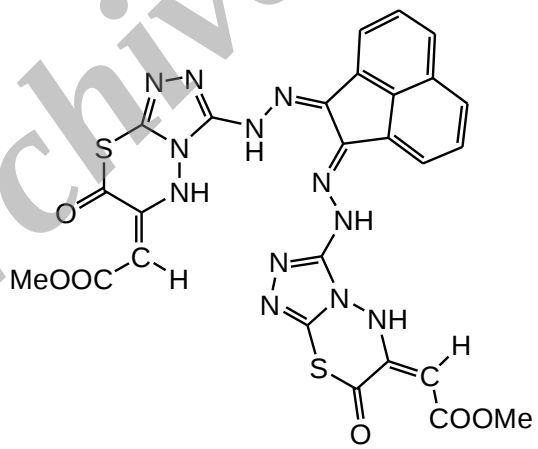
Syntihesis of 1,2,4-Triazole Derivatives and Study of the spectral properties by DFT

Navabeh nami, Ebrahim aghakhani, moohamad reza zardost*
Departmentr of chemistry, Islamic Azad University, Qaemshahr Branch , Mazandaran, Iran.

Email: Aghakhanieb@yahoo.com

In the past decade, IR spectroscopy has become important techniques for obtaining information on chemical structures and is applied in virtually all branches of chemistry. Vibrational spectroscopy is used extensively in organic chemistry for the identification of functional groups of organic compounds as well as for studies on molecular conformation,reaction kinetics, *etc* [1]. Density functional theory (DFT) has become a major tool in the methodological arsenal of computational organic chemists. For a proper understanding of IR and Raman spectra, a reliable assignment of all vibrational bands is essential.For this purpose, the quantum chemical methods, ranging from semi-empirical to DFT approaches, are invaluable tools [2], each method ha- ving its own advantages[3].

1, 2- dihydro acenaphtylidene-1, 2-dion with 4-amino-3- hydrazine - 5 - mercapto-1, 2, 4-triazole and thiosemicarbazide gave acenaphthyiene-1,2-bis-(4-amino-5-sulfanyl-4H-1,2,4-triazol-3-yl)dihydrazon and 1(2H)-acenaphthylen-thiosamicarbazone. these compounds were reacted with dimthylacetylendicarboxylate to obtain acenaphthyiene-1,2-bis-[(E)-methyl-2-(7-oxo-5H-[1,2,4]triazolo [3,4-b] [1,3,4]thiadiazin-6(7H)-yliden)acetat-3-yl]dihydrazon and acenaphthyiene-1,2-bis-[(Z)-methyl-2-(5-oxothiazolidine-4yl)acetat-3-yl]dihydrazon ,respectively in good yields. The structures determined by IR, NMR. experimental structures compared with theoretical calculated by DFT method at b3lyp/6-311G (d, p).



REFERENCES
[1] Krishnakumar, V.; Mathammal, R. *J. Raman Spectrosc*. **2009**, 40, 1599–1604.
[2] Castella-Ventura, M.; Kassab, E.; Buntinx, G.; Poizat, O. *Phys. Chem. Chem. Phys*. **2000**, 2, 4682–4689.
[3] Ushakumari, L.; Varghese, H. T.; Panicker, C. Y.; Ertan, T.; Yildiz, I . *J. Raman Spectrosc*. **2008**, 39, 1832–183