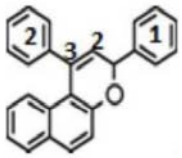
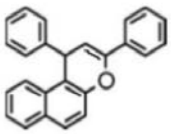
**The structure study of 1,3-diaryl-3H-benzo[f]chromenes**

M. Raeisian, M. Vakili, H. Eshghi, H. Behzadi
Department of Chemistry, Ferdowsi University of Mashhad, Mashhad 91775-1436, Iran
Department of Chemistry, Tarbiat Moallem University, Tehran, Iran
meysamraeisian@yahoo.com

There has been considerable interest in chromenes and their benzo-derivatives, not least because of their value for a variety of industrial, biological and chemical synthetic uses. In particular benzo[f]chromenes (naphthopyrans) are of special interest as photochromic compounds, electronic display system, optical switches and temporary or permanent memories [1]. Our aim in this paper, we investigate the stability and the isomer structure of diaryl-benzo[f]chromenes(I).
From the theoretical point of view, by considering the position of double bond (C2=C3) with respect to the plane of the heterocyclic ring and with respect to Ph groups, two isomers can be drawn for I (Fig. 1). The calculations of geometrical parameters and electronic energies for the isomers were performed using the Gaussian 09 program package. In this work, we applied the B3LYP level using different basis sets and MP2/6-31g** level of theory.




(a): 1,3-diaryl-3H-benzo[f]chromenes




(b):1,3-diaryl-1H-benzo[f]chromenes

Figure 1: Two possible isomer diaryl-benzo[f]chromenes.

The energy differences between two a and b isomers, calculated at the B3LYP level using different basis sets and MP2/6-31g** level of theory is at almost 5kcal/mol. But a closer look at the structure and energy value shows that isomer b is more stable than isomer a, because heterocyclic ring of the b isomer is more planar than that isomer a. According to our calculations, the dihedral angle between phenyl (1) and heterocyclic ring, on average, are 10.88 and is more than that of phenyl (2), which is in good agreement with the experimental results. The full optimized geometrical parameters of 1,3-diaryl-3H-benzo[f]chromenes isomers are in excellent agreement with the results of the experimental structures [3] nearly in the experimental error range.

**References**

**[1]** J.S. Yadav, B.V.S. Reddy, S.K. Biswas, et al. Tetrahedron Lett. 50 (2009) 5798.
**[2]** H.Eshghi ,*, GHZohuri, s.Damavandi ,m.Vakili.Chinese Chemical Letters 21 (2010) 1423–1426
**[3]** XiaobingXu, Jun Liu,Linfeng Liang, H. Li,and Y.Lia,*Adv. Synth. Catal. 2009, 351, 2599 – 2604