Poster Presentation

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Molecular structure investigation by ab initio, DFT and X-ray diffraction of thiazole-derived compound

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We report here the synthesis of Z-3-(2-Ethoxyphenyl)-2-(2-Ethoxyphenyl)-1,3-Thiazolidin-4-one compound. The crystal structure has been determined by X-ray diffraction. The compound crystallizes in the monoclinic system with space group P21/n and cell parameters: a = 9.4094(10), b = 9.3066(10), c = 20.960(2) Å, β=99.0375(10)°, V = 1812.7(3)Å3 and Z = 4. The structure has been refined to a final R = 0.05 for 2083 observed reflections. The refined structure was found to be significantly non planar. The molecule exhibits intermolecular hydrogen bond of type C–H…O, C–H…N and C–H…S. Ab initio calculations were also performed at Hartree–Fock and density functional theory levels. The full HF and DFT geometry optimization was carried out using 6-31G(d,p) basis set. The observed molecular structure is compared with that calculated by both HF and density functional theory methods. The optimized geometry of the title compound was found to be consistent structure determined by X-ray diffraction.

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