Poster Presentations

[MS24-P38] Experimental and theoretical studies on a novel of a [3,2-α]pyrimidine derivate

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The title molecule, ($C_{30}H_{34}N_2O_2S1$), was synthesized and characterized by single-cyrstal X-ray diffraction. The compound cyrstallizes in the triclinic space group *P*21/c. In addition, the molecular geometry, vibrational frequencies and frontier molecular orbitals analysis of the title compound in the ground state have been calculated by using the HF/6-31G(d) and B3LYP/6-31G(d) methods. Molecular electrostatic potential of the compound was also performed by the theoretical method.

Keywords: X-ray, ab-initio calculations.