# DFT STUDY OF (2Z,3Z)-1,4-DITHIANE-2,3-DIONEDIOXIME

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| **ABSTRACT**  In this study, electronic structures vicinal dioxime were studied by DFT calculations. Structural and electronic parameters of the complexes were determined by using Gaussian 09 program. First of all, geometric parameters (bond length, bond angle, torsion angle) of the most stable form of the complex were determined with mPW1PW91 iop(3/76=0572004280) / gen [S: cc-pvqz, C and H: 6-31+g(d,p), N: 6-31+g(2d), O: cc-pvqz] level. The theoretical frontier molecular orbital descriptors such as electronegativity, chemical potential, softness, electrophilicity index, and electron affinity of the title compound were calculated with the same level. In addition, the total and partial density of state distribution (TDOS, PDOS) of the molecular orbitals, molecular electronic potential surface map (MEP) and nonlinear optical properties (NLO) of the compound were determined. |

# Keywords: Vicinal dioxime, Density Fuctional Theory, MEP, Nonlinear optics.