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Synthesis and Electronic Structure of New Aryl- and Alkyl-Substituted 1,3,4-Oxadiazole-2-thione Derivatives

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Abstract: New 5-alkyl and 3-(2,4-dimethylphenyl) substituted 1,3,4-oxadiazole-2-thione derivatives were synthesized by the ring closure reactions of various acylhydrazides with carbon disulphide. Mannich bases for some of these compounds were also synthesized by condensation with benzaldehyde and primary amines. All new compounds were characterized by spectral data. Most of them were tested for their antibacterial and antituberculostatic activity. Molecular orbital calculations at the HF/6-31G** level were also performed to determine the optimized geometrical structures. Results indicated electron delocalization over several atoms of the ring. An additional study on the tautomeric equilibrium between 1,3,4-oxadiazole-2-thione and its thiol form showed that the thione tautomer is favoured by 9.616 kcal/mole in the gas phase and by 12.123 kcal/mole in aqueous medium.

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