OXAZIRIDINE (C-CH_3NO), C-CH_2NO RADICALS AND CL, NH_2 AND METHYL DERIVATIVES OF OXAZIRIDINE; STRUCTURES AND QUANTUM CHEMICAL PARAMETERS

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Abstract. Oxaziridine [c-CH_3NO (X^1A)], c-CH_2NO (X^2A) radicals and Cl, NH_2 and methyl derivatives of oxaziridine structures have been optimized via DFTB3LYP level of theory using 6-311++G (d, p) basis set. Population analysis had been carried out. Vertical ionization energy (*VIE*) and adiabatic ionization energy (*AIE*), Fukui indices and some quantum chemical parameters were calculated. N-O bond was determined as weakest bond in oxaziridine triangle. The effect of electron withdrawing and electron donating groups on stability of weakest bond were assessed.

Keywords: oxaziridine, DFT, Fukui function, vertical ionization energy, adiabatic ionization energy.

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