ABSTRACT

Novel derivatives of 5-Aminotetrazole were synthesized and characterized using proton-NMR, IR spectrophotometer and CHNS analyzer and single crystal X-ray diffractometer studies. The compounds were further studied using computational methods. The compounds were prepared following conventional method, reported in literature. Consequently new reactants were used employing conventional techniques. In the IR spectra, the band due to C--N group, which is present in all studies compounds, was observed at about 1030-1150 cm^{-1}. In ^{1}H NMR spectra, aromatic protons were observed at about δ 7.4 to 7.9 ppm in all derivatives. The geometric and electronic properties have been investigated by density functional theory. The distribution patterns of highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) of the systems have been studied in the S_0 states. The optimized parameters are in good agreement with experimental data which showed that adopted method is reliable and accurate.