**ABSTRACT**

 In this study the tautomerism of 1H-imidazole-4,5-tetrazole (HIT) are investigated in liquid and gas phases using density functional theory. The intramolecular hydrogen bond proves to be the key factor for the stability and the chemical properties of the tautomers. Boltzmann population analysis shows that the probability for the existence of the most stable tautomers is prominent in both gas and liquid phases. The dipole moment of all the tautomers increases with increase in polarity of the medium considered. 15N NMR and 13C NMR chemical shift along with MESP predict that the nitrogen atoms in both tetrazole and imidazole rings are excellent metal coordination sites. The pKa value predicts that the tautomers to be acidic in nature. A linear relationship between the redox potential and the ionization potential shows that all the tautomers tend to lose electrons, hence can coordinate with metals strongly.