Theoretical studies on the structure and hydrogen bonding of 8-amino-1-naphthol and its one water complex. El-Rayyes, Ali A.; Htun, Than. Department of Chemistry, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia.

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Abstract

Geometry and structure of 8-amino-1-naphthol (8-AN) has been studied theor. in the ground and excited states and in solvents. Ground state calcns. were carried out at DFT/6-31G and the excited state geometries were calcd. at RCIS/3-21G level of theory. The mol. is found to exist in two forms, the cis (where the -OH group is directed towards the amino nitrogen) and the trans forms with the cis to be the most stable structure. Evidence for an intramol. hydrogen bonding is found. Calcns. on solvent effect further support the presence of intramol. hydrogen bonding and showed the possibility of proton transfer via the assistance of solvent mol.