https://www.researchgate.net/publication/304452036_Study_of_Proton_Transition_and_quantum-chemical_calculations_for_1_8-bis_N_N-dimethylamino_naphthalene_DMAN_and_derivatives_by_Hyperchem_program

THEORETICAL STUDY OF PROTON TRANSFER FOR 1,8-BIS(N,N-DIMETHYLAMINO)NAPHTHALENE (DMAN) BY HYPERCHEM PROGRAM

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ABSTRACT: Proton Sponge , 1,8-bis(N,N-dimethylamino)naphthalene, was optimized and studied as a strong base to find the ability for N-to-N proton transfer and the effect of adding substituents groups to Proton Sponge considering it as a original compound. All calculations, Total Energy, Energy of Transition State, Proton Affinity, Microwave Frequency and Intensity have been carried out by using HyperChem8.0 package. The most effect on increase Proton Affinity appeared by adding methyl group at para while the most effect on decrease it by adding fluoride at mata. In same time adding (O-(C=O)-O-Phenyl) group at para have the most effect on increase Energy of Transition State while adding chloride at para have the most effect on decrease it.