

SPECTROSCOPY AND BRAIN CHEMISTRY OF SEROTONIN AND DOPAMINE CONFORMERS

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The neurotransmitters Serotonin and Dopamine are thought to play a distinct role in brain chemistry and human behavior. In the Present work we will discuss the Conformer specific spectroscopic signatures of protonated Serotonin and Dopamine in the gas phase and aqueous media. A comparison of the computed frequencies of protonated Dopamine with the observed Raman spectrum indicates that gauche and trans conformers coexist in the liquid dopamine and exhibit population redistribution upon a change in pH during stress. Since the trans-conformers have more affinity for the receptor site than the gauche conformers, the higher population distribution of trans conformers is hypothesized to be associated with efficient neurotransmission and normal human behavior. The strong cation- π interaction in the isolated gauche conformers of serotonin in the gas phase is predicted to be a possible cause of human aggression. 1. Vipin Bahadur Singh, ACS Chem Neuroscience, 12,613-625 (2021)