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Theoretical Study of the Dopaminephotochemical Behaviour

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The equilibrium geometry structures and photochemistry properties of the dopaminehave been investigated using the density functional theory in both ground and excitedstates. The efficiency of different hybrid and meta-hybrid DFT exchange-correlationfunctionals has been testing using CCSD level of theory as reference. The bonds be-tween different carbon, oxygen and nitrogen atoms have been analyzed for nine differentdopamine derivatives. The light induced properties such as the fluorescence rate andabsorbtion efficiency have been calculated for all the structures using DFT methods