

Abstract

A molecular inclusion complex of a diacetylene and porphyrin ring is chosen as a model to check if it can be a potential light emitter as in the case of an ammonia molecule. In this work, it is shown that a supramolecular complex of diacetylene threaded porphyrin is a stable minimum with a very high dipole moment of 4.45 Debye at B3LYP/6-311+g(d,p). Although the system is thermodynamically unfavorable, there are remote possibilities of kinetic trapping in a well of depth 11.4 kcal/mol. The barrier for insertion was calculated to be 110.29 kcal/mol. The neutral species corresponding to the same structure has a higher dipole moment and similar potential energy surface (PES) characteristics