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Title:	Molecular Machines as Light Emitters : A Porphyrin-Diacetylene System
Authors:	Singh, Nitin Kumar (/jspui/browse?type=author&value=Singh%2C+Nitin+Kumar)
Keywords:	Chemistry Porphyrin Ring Diacetylene
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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
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