

Multiple Hydrogen Bond Tethers for Grazing Formic Acid in Its Complexes with Phenylacetylene

Ginny Karir*, Gaurav Kumar¹, Bishnu Prasad Kar² and K. S. Viswanathan*
Department of Chemical Sciences, Indian Institute of Science Education and Research,
Sector 81, Mohali 140306, Punjab, India

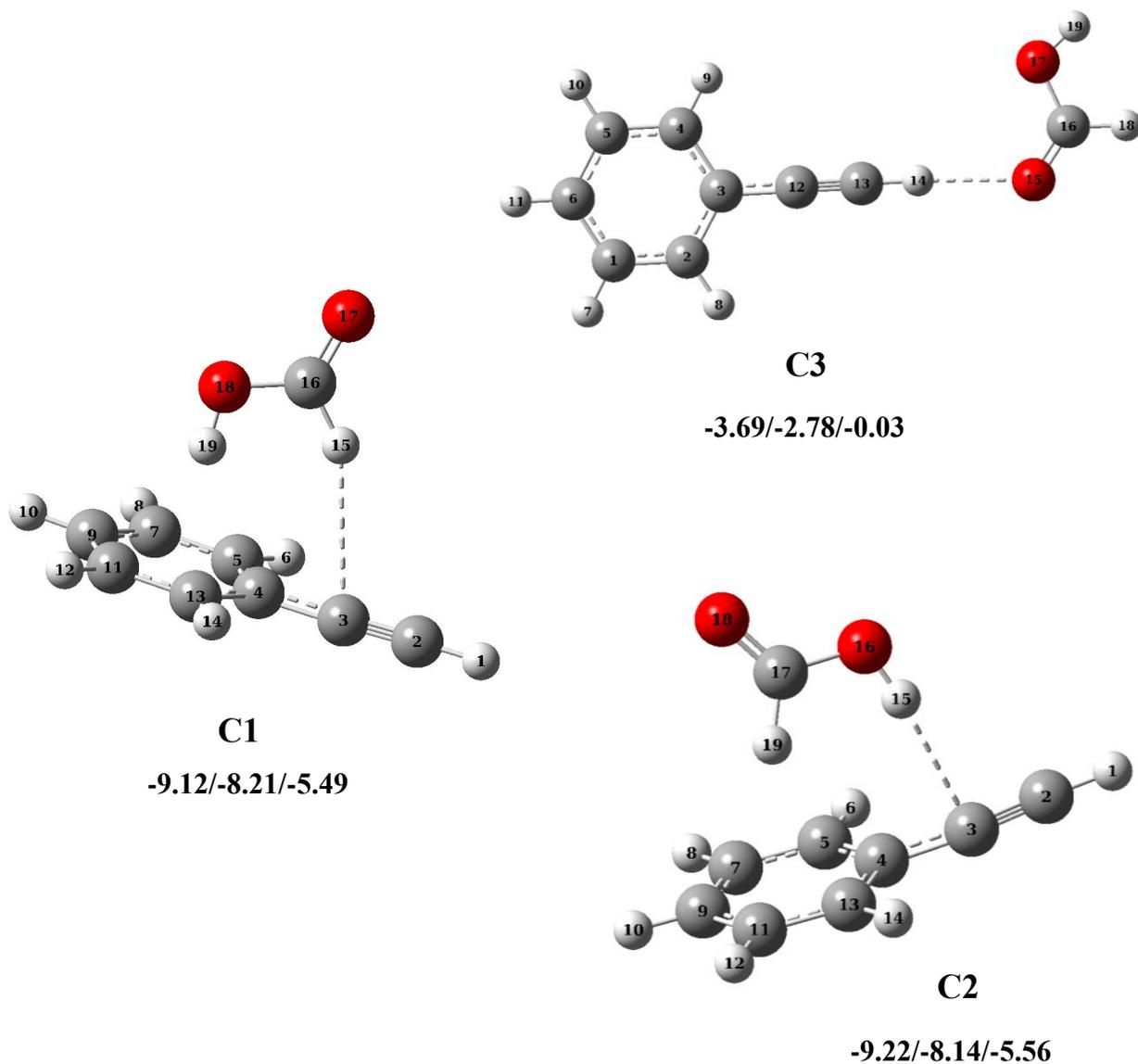


Figure S1. Optimized structures of PhAc-cFA computed at the MP2/aug-cc-pVDZ level of theory. Interaction energies computed at the same level of theory are given as Uncorrected/ZPE corrected/BSSE Corrected energies in kcal/mol.